

FIG. 1

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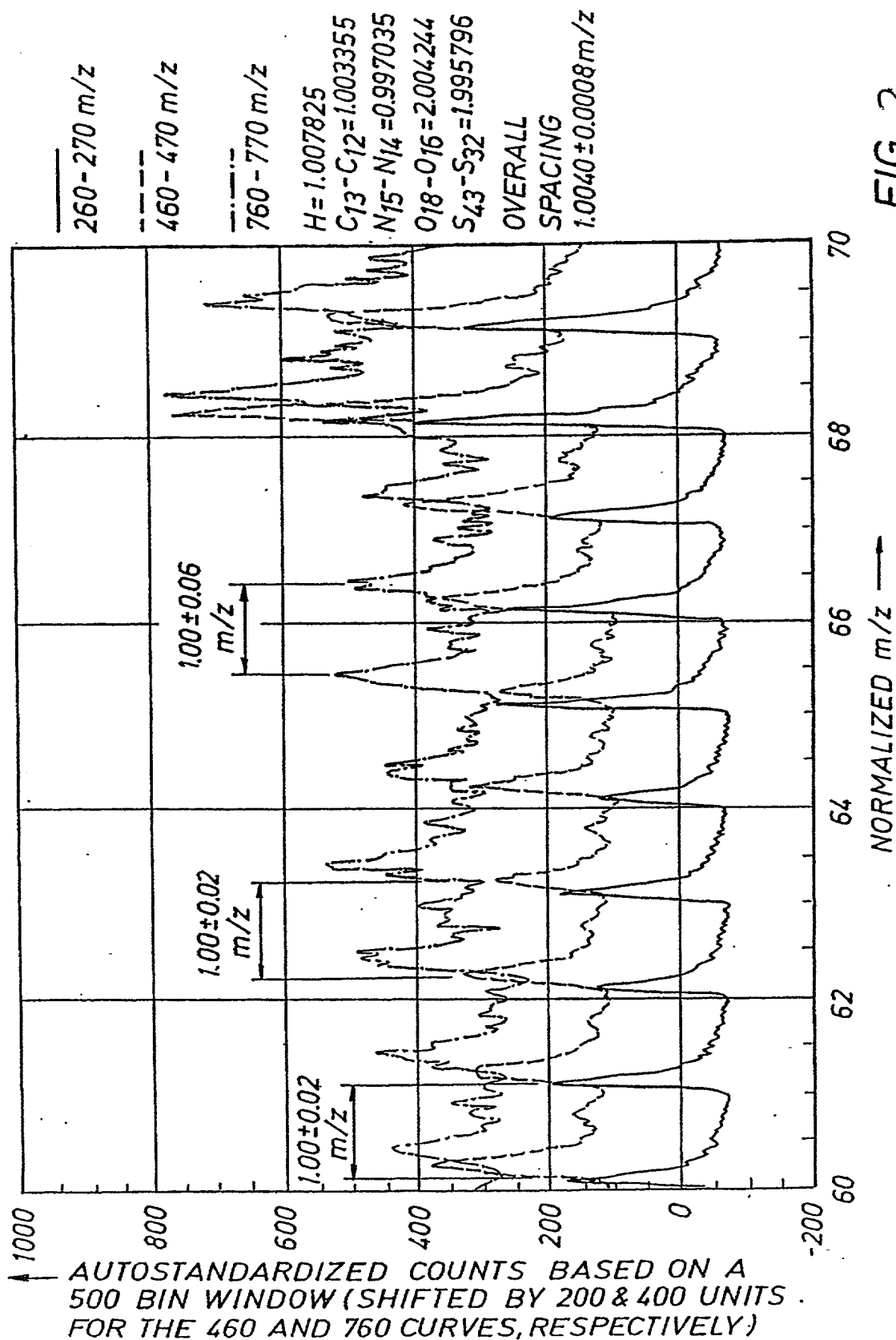


FIG. 2

+

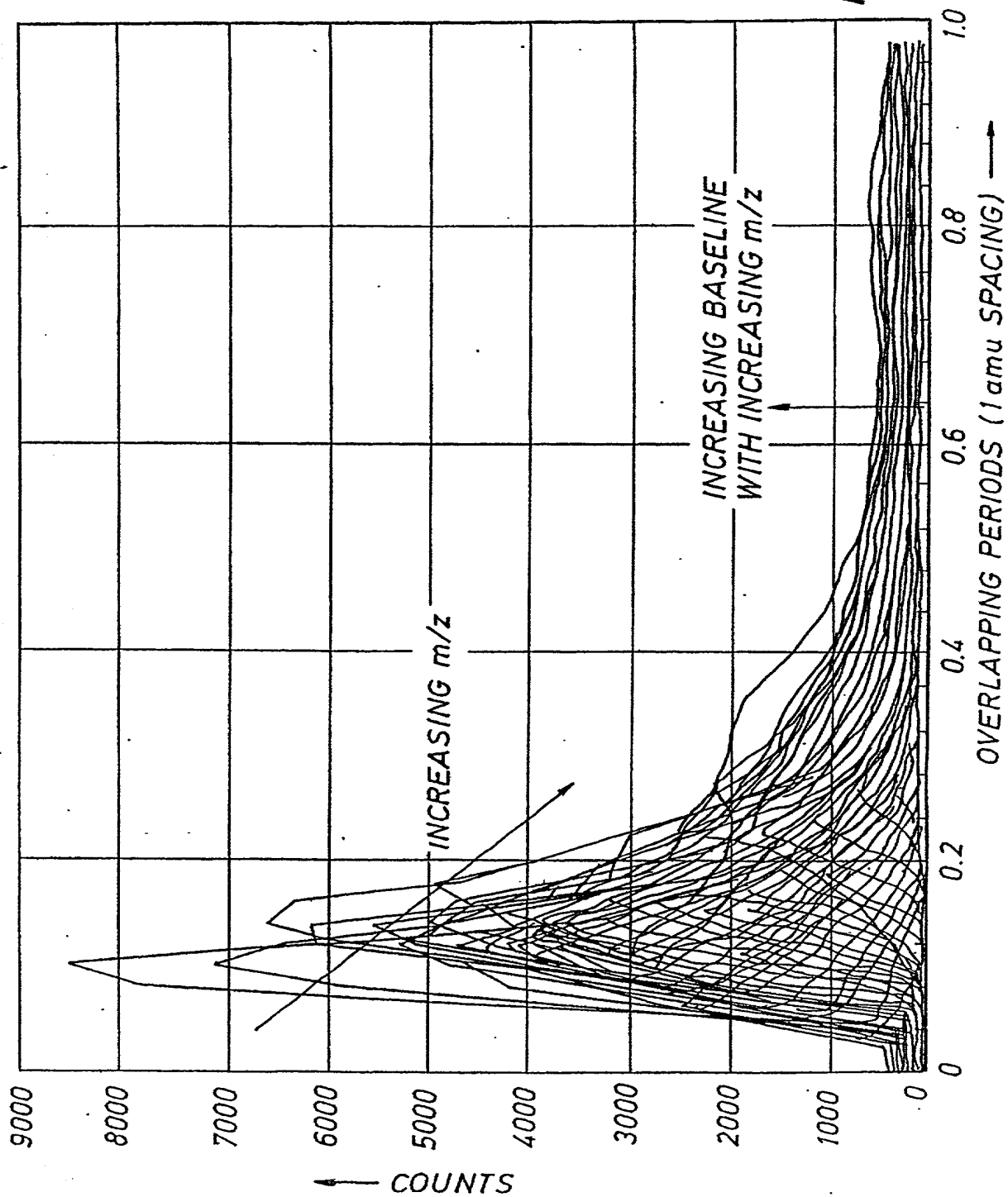


FIG. 3

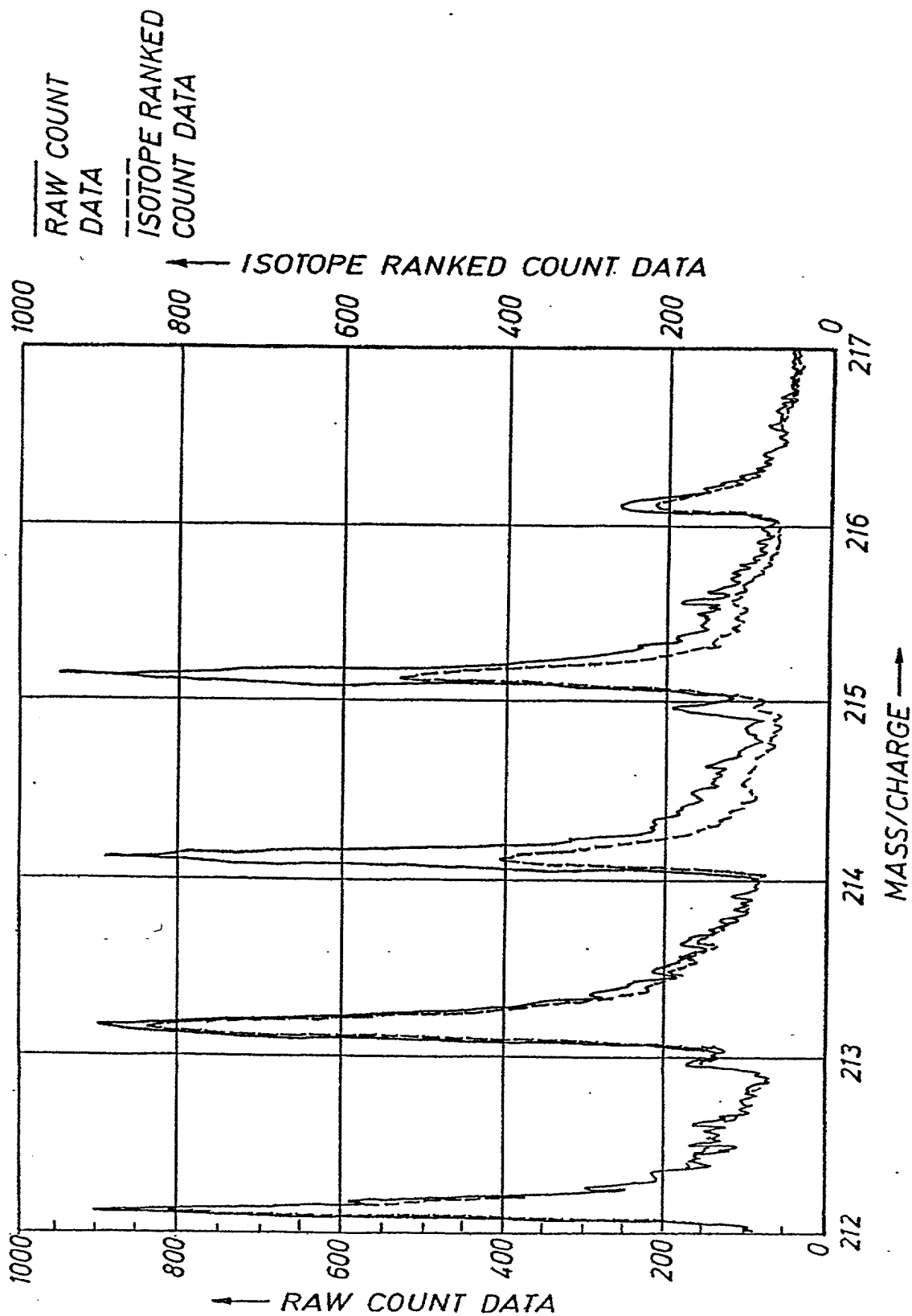


Fig. 14

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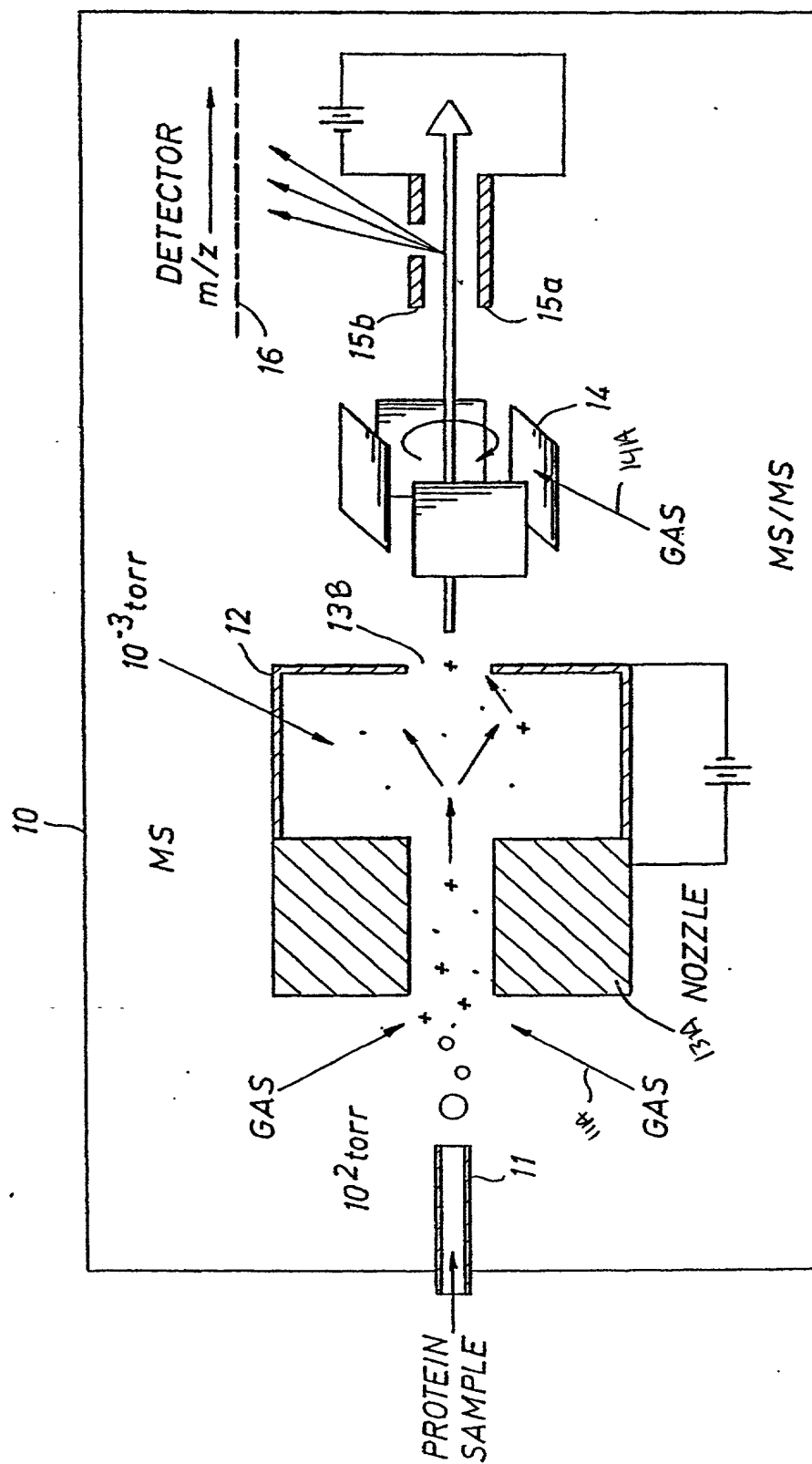


FIG. 5

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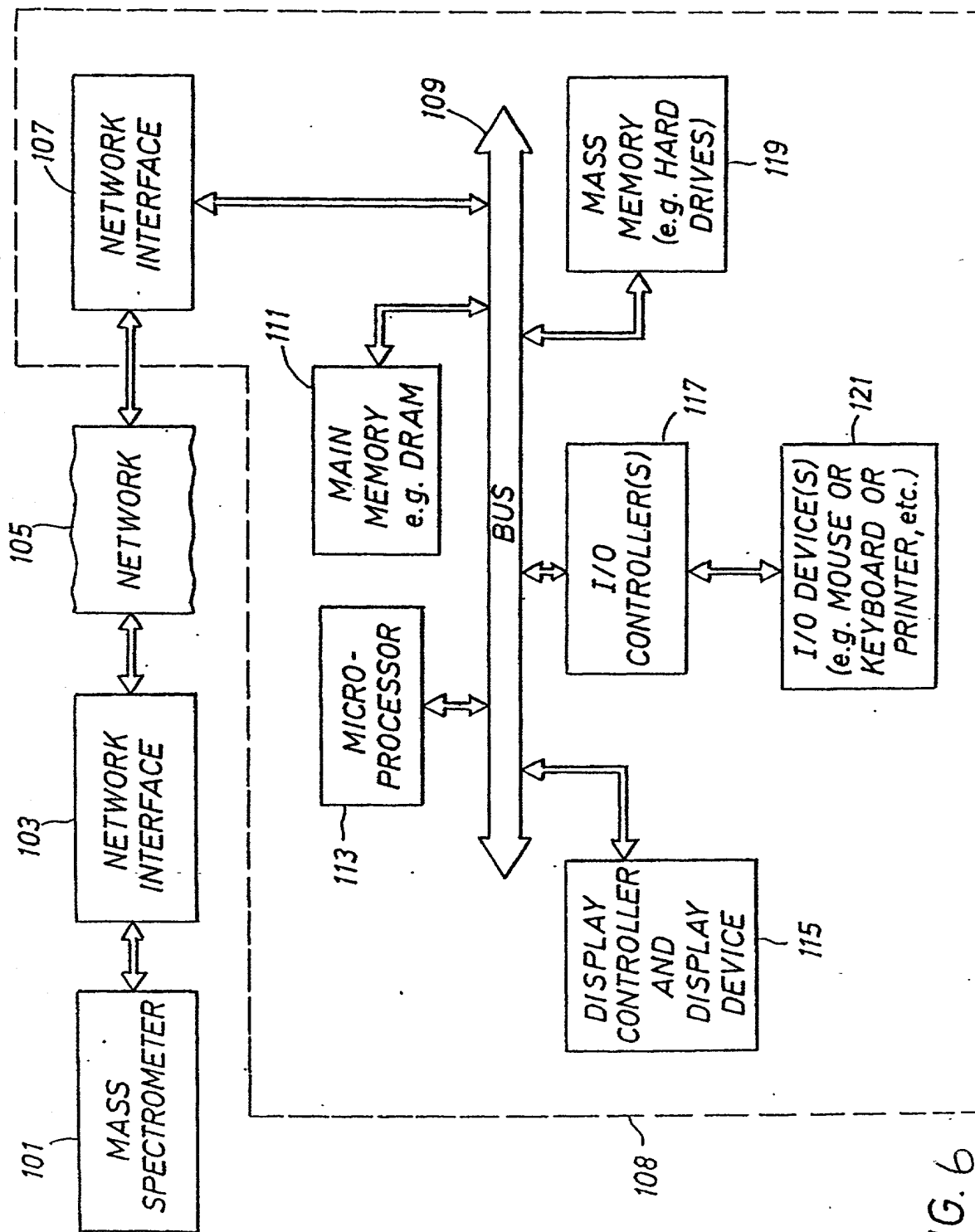


FIG. 6

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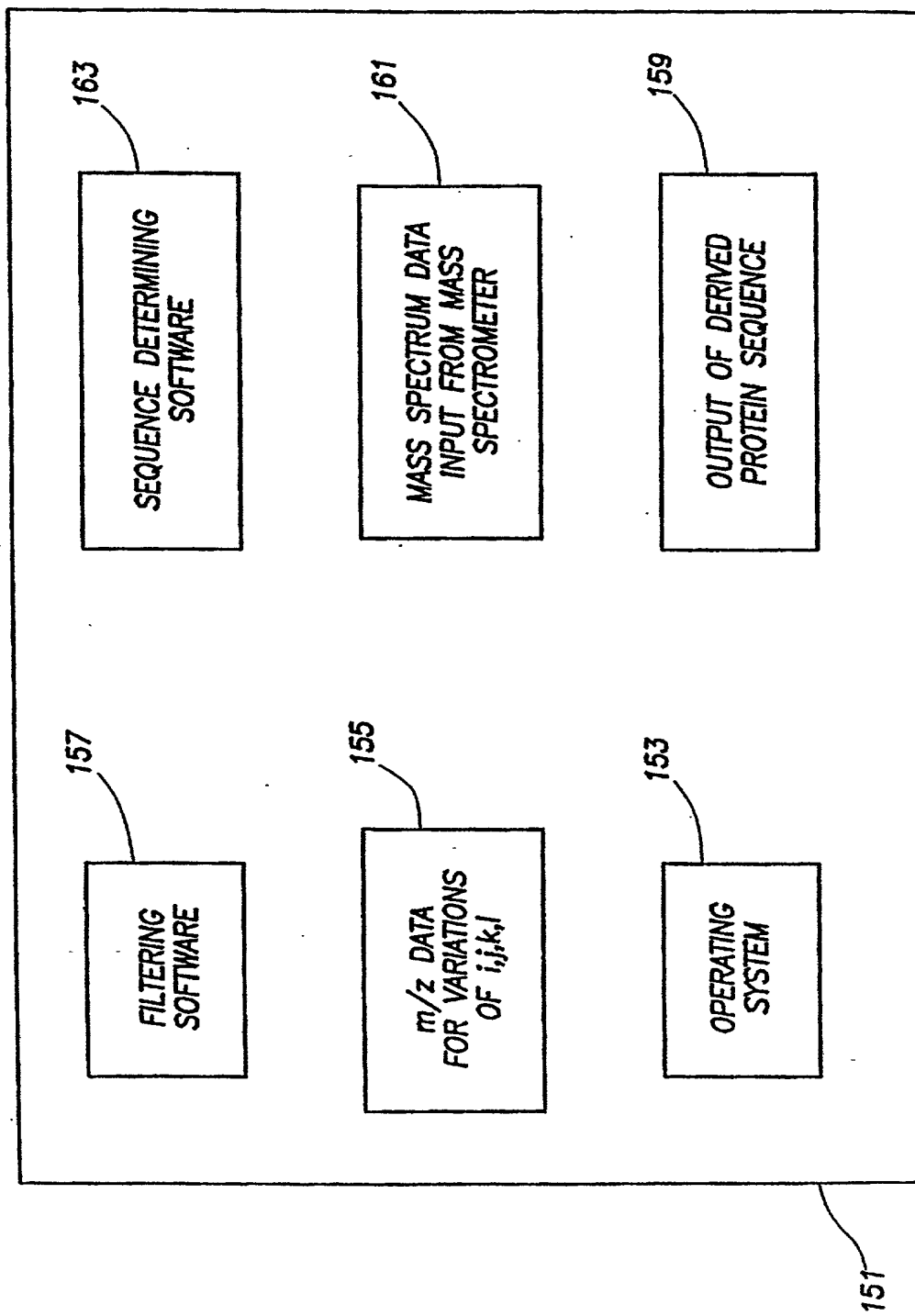
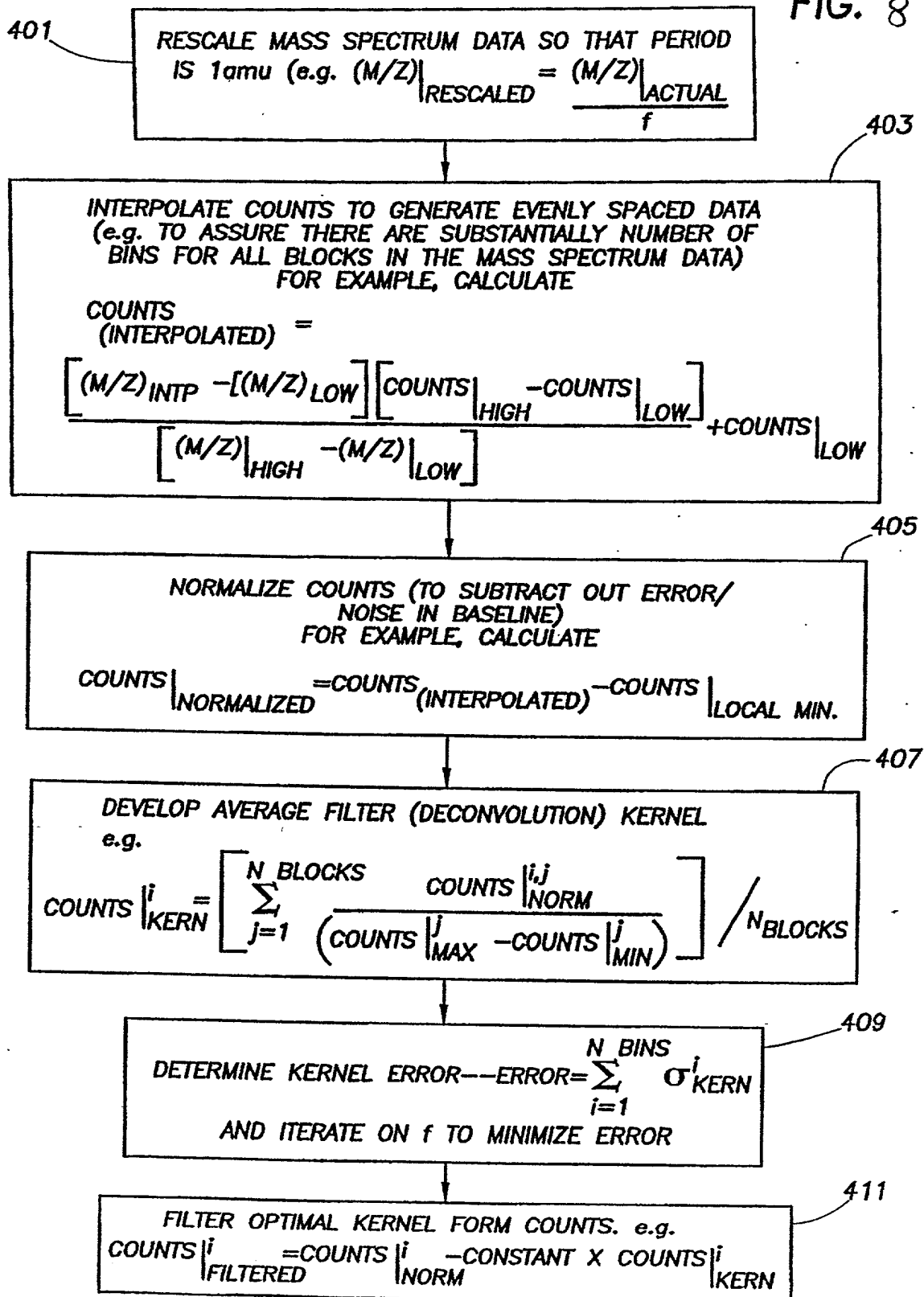


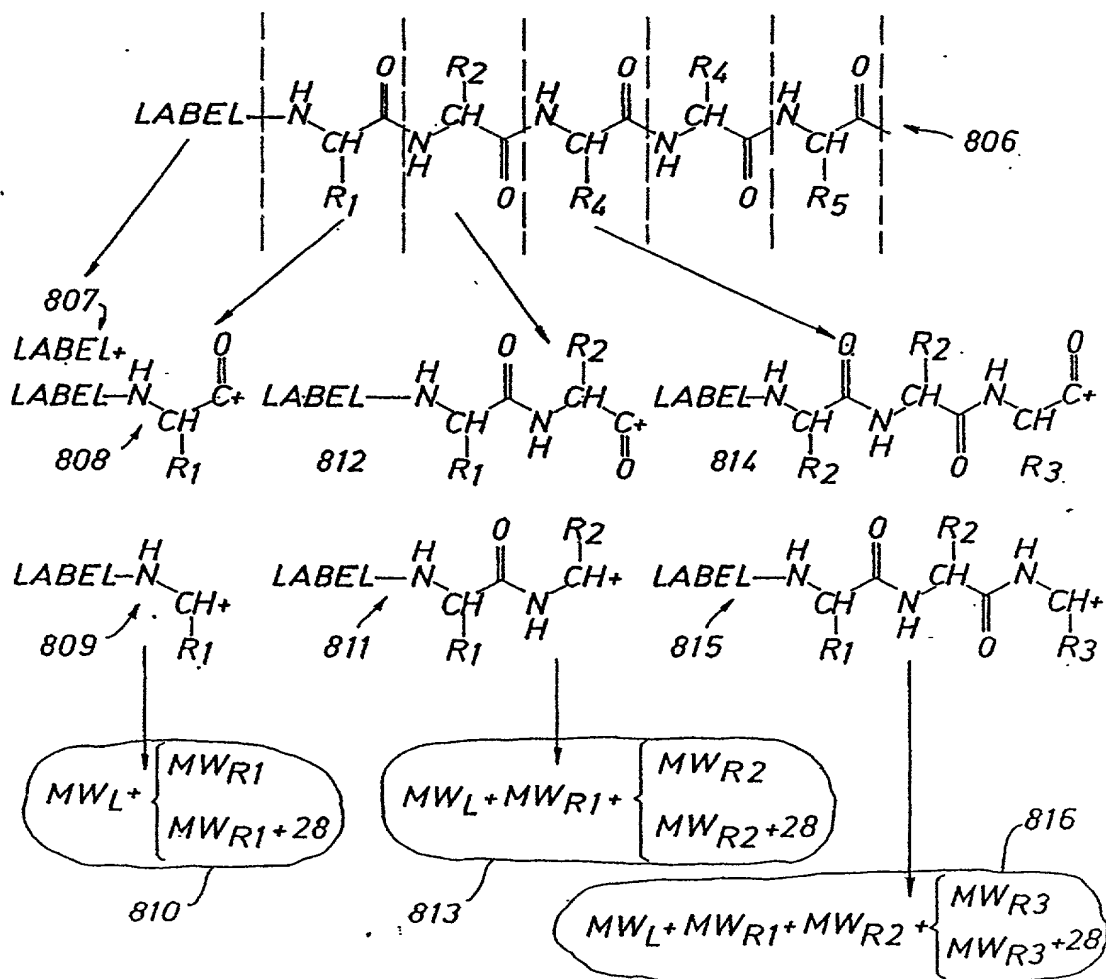
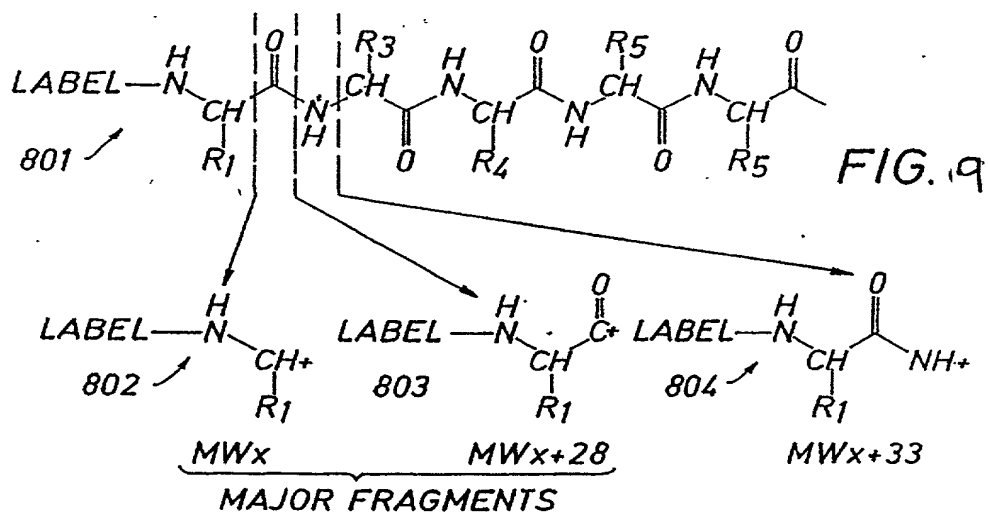
FIG. 7

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FIG. 8







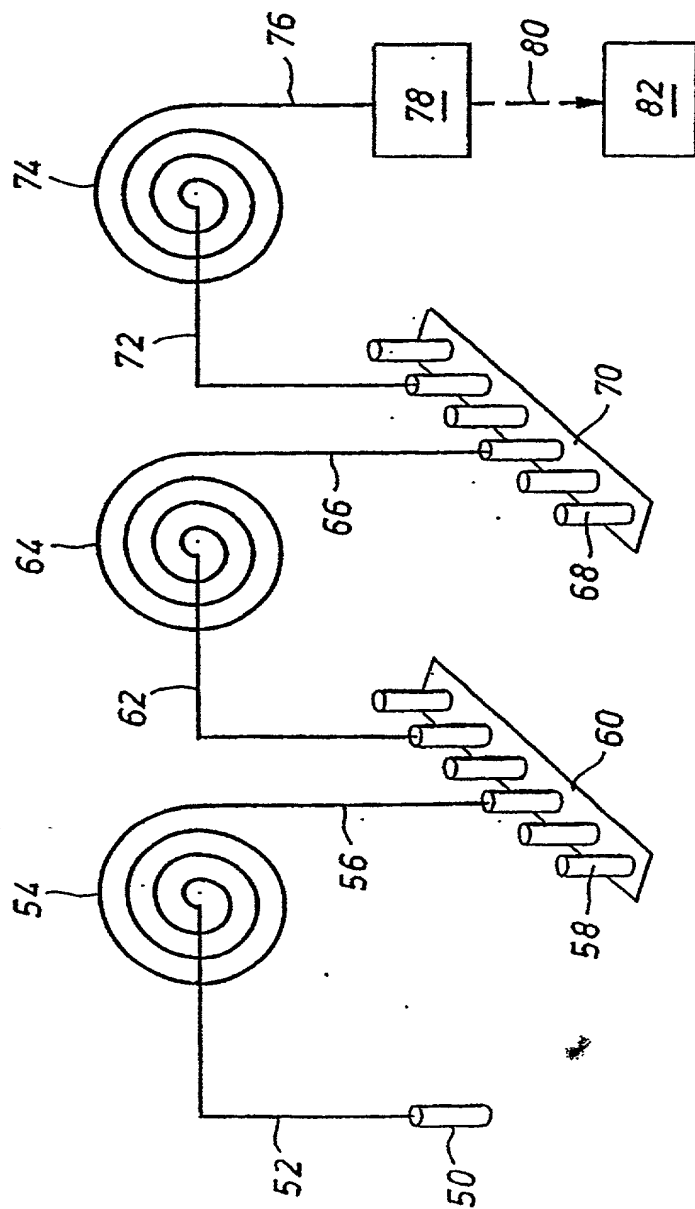


FIG. 10

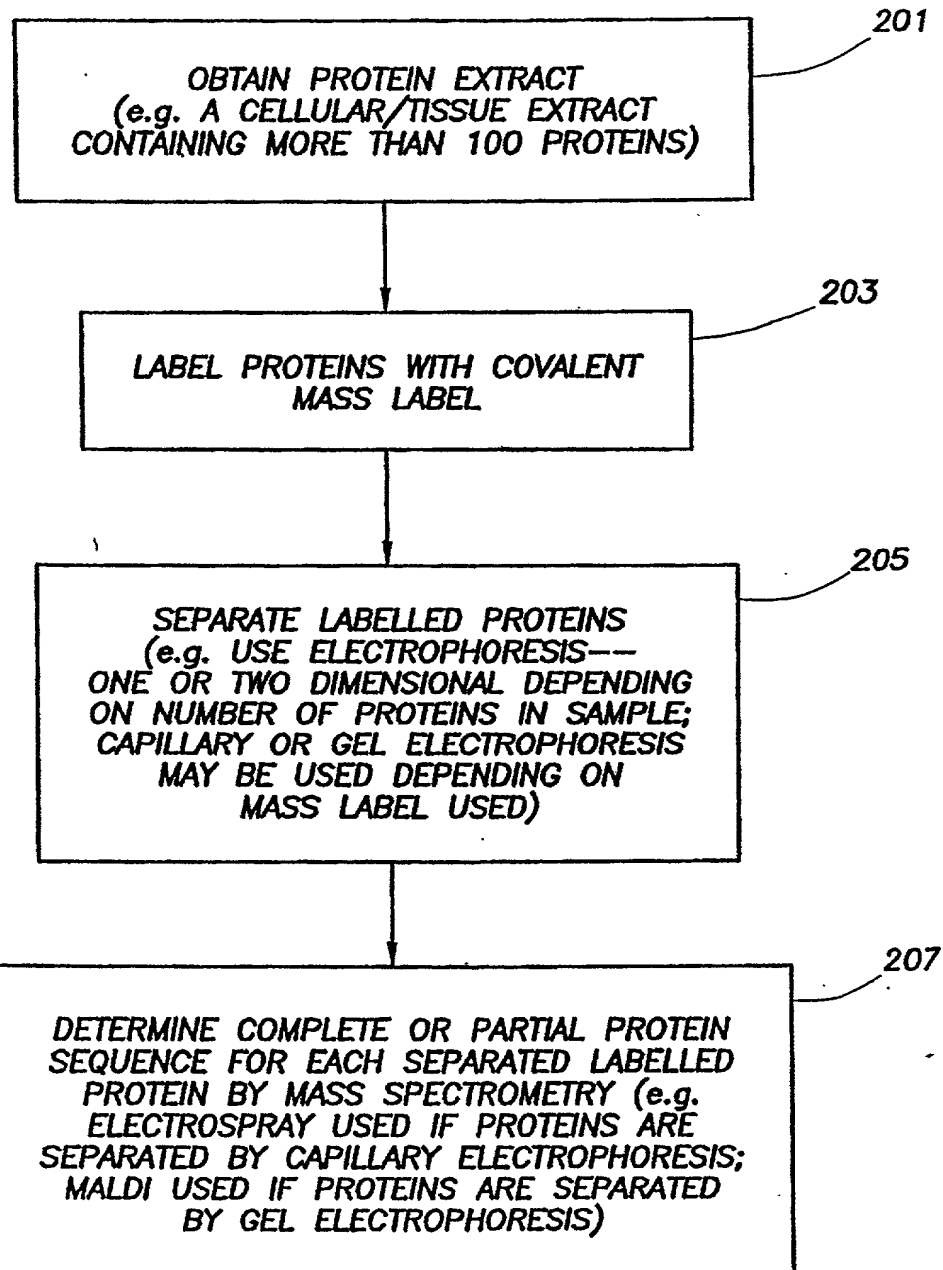


FIG. 11

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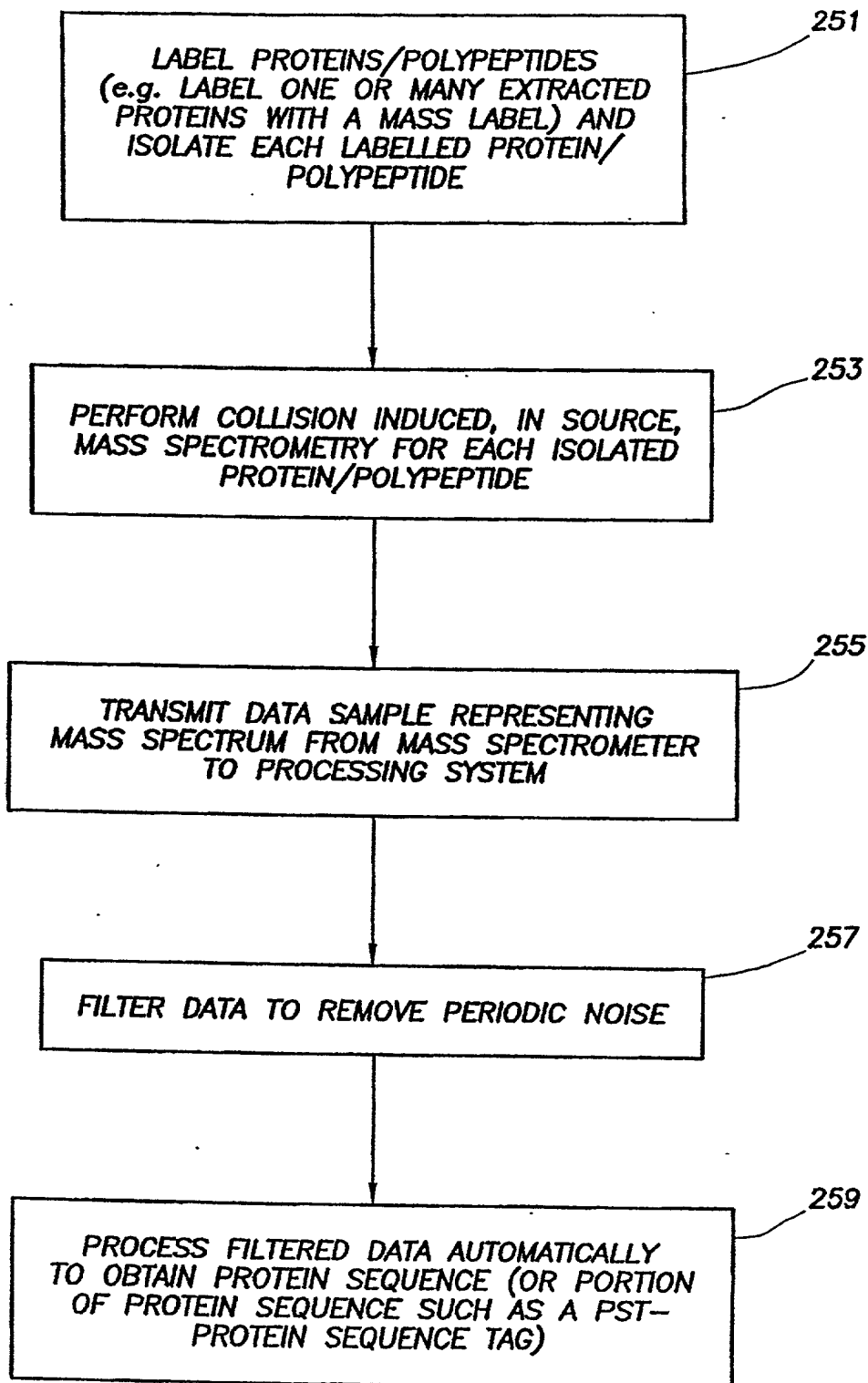


FIG. 12

TOP SECRET

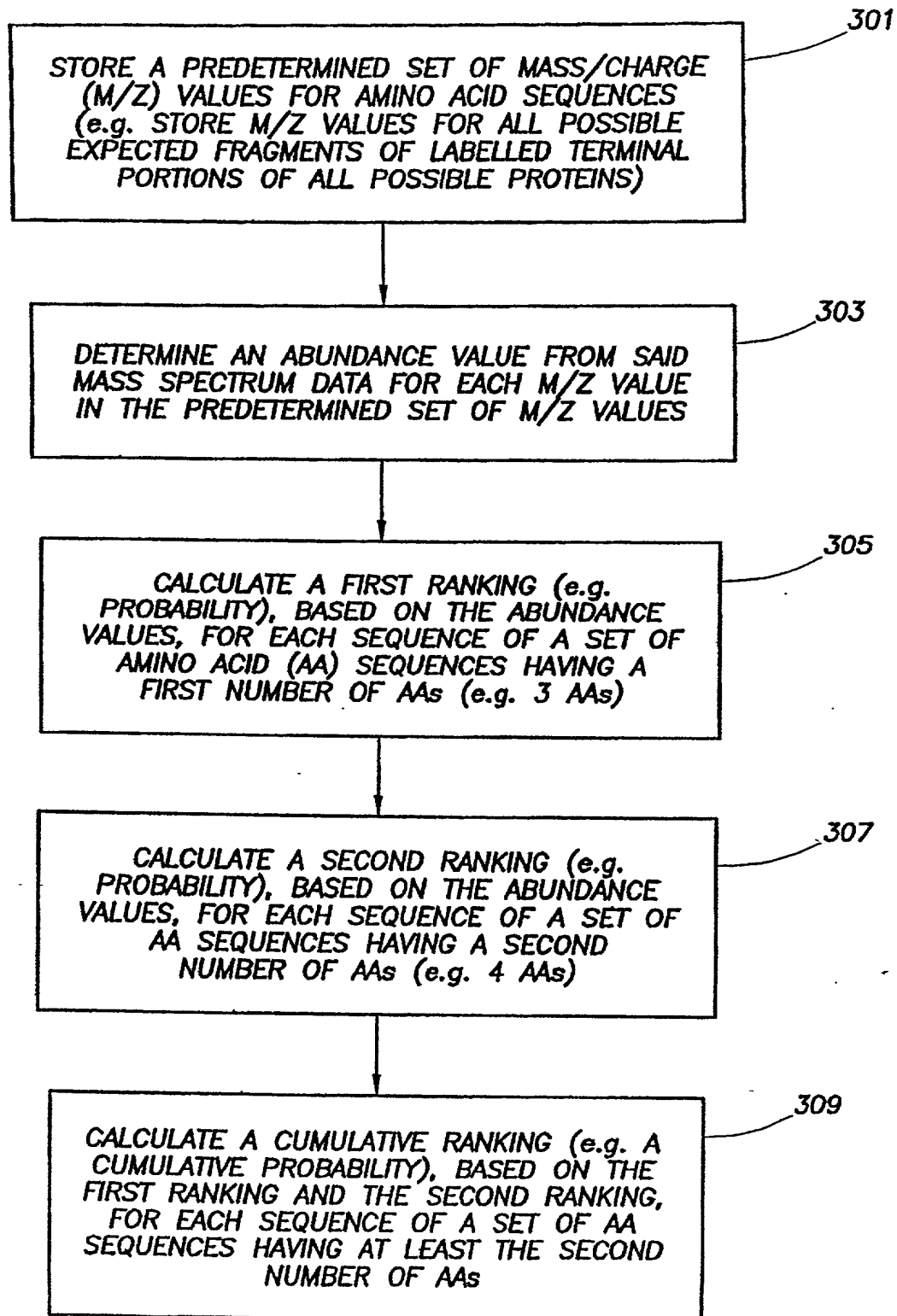


FIG. 13

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FIG. 14A

FOR EACH POSSIBLE EXPECTED FRAGMENT OF A TERMINALLY LABELLED SEQUENCE OF AAs, PERFORM LOOKUP IN MASS SPECTRUM DATA FOR ABUNDANCE VALUE AT M/Z VALUE OF POSSIBLE EXPECTED FRAGMENT (e.g.  $C_{i,j,k,l} = \text{LOOKUP} [(M/Z)_{i,j,k,l}]$ )

DETERMINE MASTER COUNT, FOR EACH PARTICULAR POSSIBLE SEQUENCE, OVER ALL POSSIBLE ION TYPES AND CHARGE STATES FOR PARTICULAR SEQUENCE

e.g.

$$C_{i,j}^M = \sum_{\substack{\text{MAX} \\ \text{CHARGE} \\ \text{STATES} \\ I=\text{MIN} \\ \text{CHARGE} \\ \text{STATES}}} \left( \sum_{\substack{\text{MAX} \\ \text{ION} \\ \text{TYPES} \\ k=1}} C_{i,j,k,l} \right)$$

WHERE

$i$ =NUMBER OF AMINO ACIDS (AAs) IN SEQUENCE  
 $j$ =NUMBER OF POSSIBLE SEQUENCES (USUALLY,  $19^i$ )  
 $l$ =NUMBER OF ION TYPES FOR EACH RESIDUE  
 (e.g. ION TYPES a,b, AND POSSIBLY c AT N TERMINUS AND ION TYPES x,y, AND POSSIBLY z AT C TERMINUS)  
 $k$ =NUMBER OF CHARGE STATES FOR EACH ION TYPE

FOR EACH MASTER COUNT ( $C_{i,j}^M$ ) FOR A PARTICULAR POSSIBLE SEQUENCE AT A GIVEN SEQUENCE LENGTH, COMPARE THE MASTER COUNT TO ALL OTHER MASTER COUNTS FOR ALL OTHER POSSIBLE SEQUENCES FOR THE GIVEN SEQUENCE LENGTH TO PRODUCE A RANKING OF MASTER COUNTS OF ALL POSSIBLE SEQUENCES AT THE GIVEN LENGTH OF AAs. FOR EXAMPLE, THE COMPARISON MAY BE A RANKING OF PROBABILITIES WHERE EACH PROBABILITY IS A PROBABILITY OF A PARTICULAR SEQUENCE AT THE GIVEN SEQUENCE LENGTH RELATIVE TO ALL OTHER POSSIBLE SEQUENCES AT THE SAME LENGTH

TO FIG. 14B

FIG. 14 B

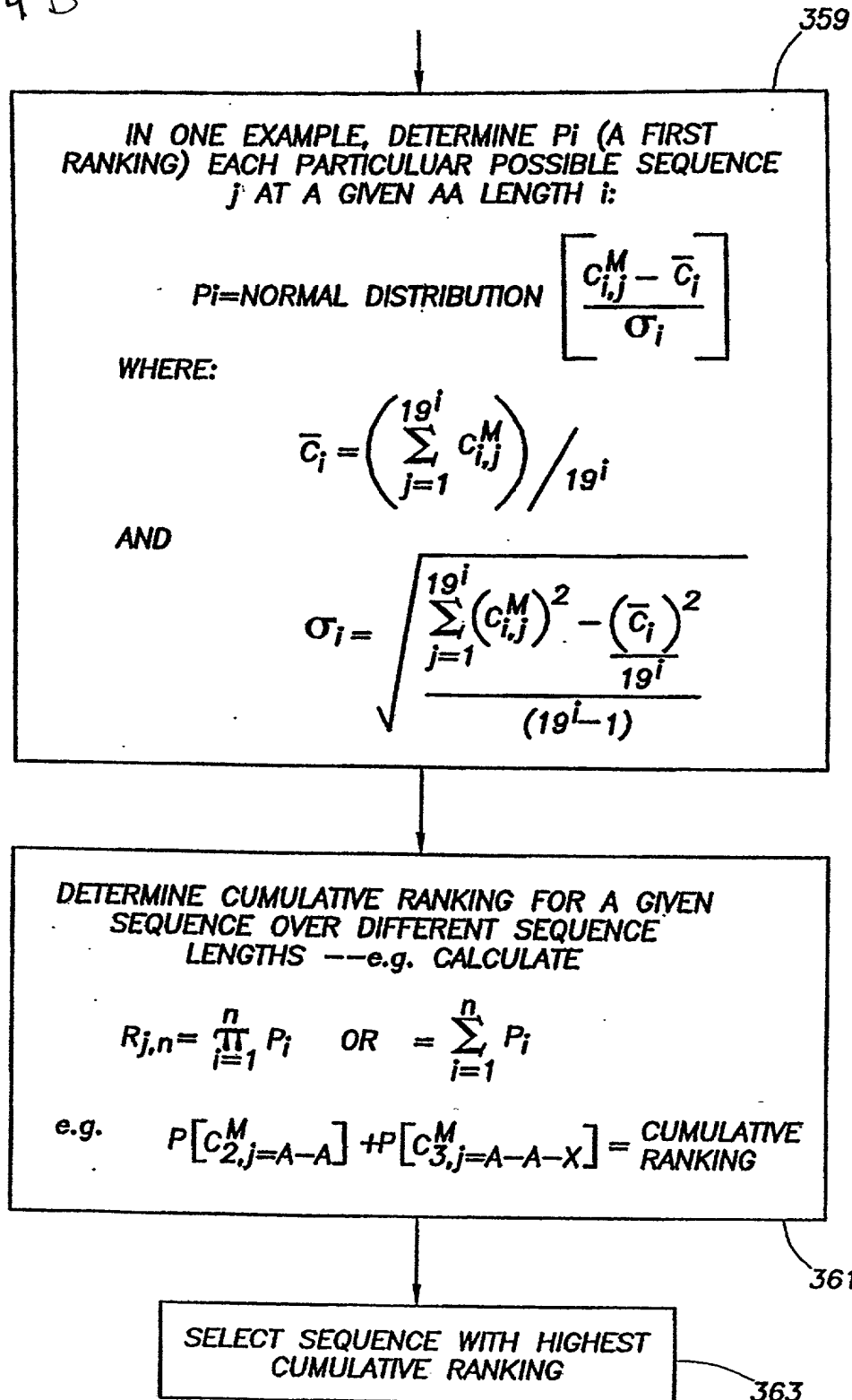


FIG. 15

FIG. 15

FIG. 15

1101  $C_{i,j,k,l} = \text{LOOKUP}[(m/z)_{i,j,k,l}] \text{ LABEL 1}$

1103  $C_{i,j} = \sum_{k=\min}^{\text{MAX CHARGE STATES}} \sum_{l=1}^{\text{MAX ION TYPES}} C_{i,j,k,l}$

1105  $\bar{C}_i = \frac{\sum_{j=1}^{19^i} C_{i,j}}{19^i}$

1107  $\sigma_i = \sqrt{\frac{\sum_{j=1}^{19^i} C_{i,j}^2 - \left( \sum_{j=1}^{19^i} C_{i,j} \right)^2}{(19^i - 1)}}$

1109  $P_i = \text{NORMDIST} \left[ \frac{(C_{i,j} - \bar{C}_i)}{\sigma_i} \right]$

1111  $R_{j,n} = \prod_{i=1}^n P_{i,j} \text{ OR } \sum_{i=1}^n P_{i,j}$

1121  $d_{i,j,k,l} = \text{LOOKUP}[(m/z)_{i,j,k,l}] \text{ LABEL 2}$

1123  $D_{i,j} = \sum_{k=\min}^{\text{MAX CHARGE STATES}} \sum_{l=1}^{\text{MAX ION TYPES}} d_{i,j,k,l}$

1125  $\bar{D}_i = \frac{\sum_{j=1}^{19^i} D_{i,j}}{19^i}$

1127  $\sigma_i^{\text{label2}} = \sqrt{\frac{\sum_{j=1}^{19^i} D_{i,j}^2 - \left( \sum_{j=1}^{19^i} D_{i,j} \right)^2}{(19^i - 1)}}$

1129  $q_i = \text{NORMDIST} \left[ \frac{(D_{i,j} - \bar{D}_i)}{\sigma_i^{\text{label2}}} \right]$

1135  $R_{j,n} = \prod_{i=1}^n (p_i q_i) \text{ OR } \sum_{i=1}^n (p_i q_i)$

1131  $R_{j,n} = \prod_{i=1}^n q_i \text{ OR } \sum_{i=1}^n q_i$



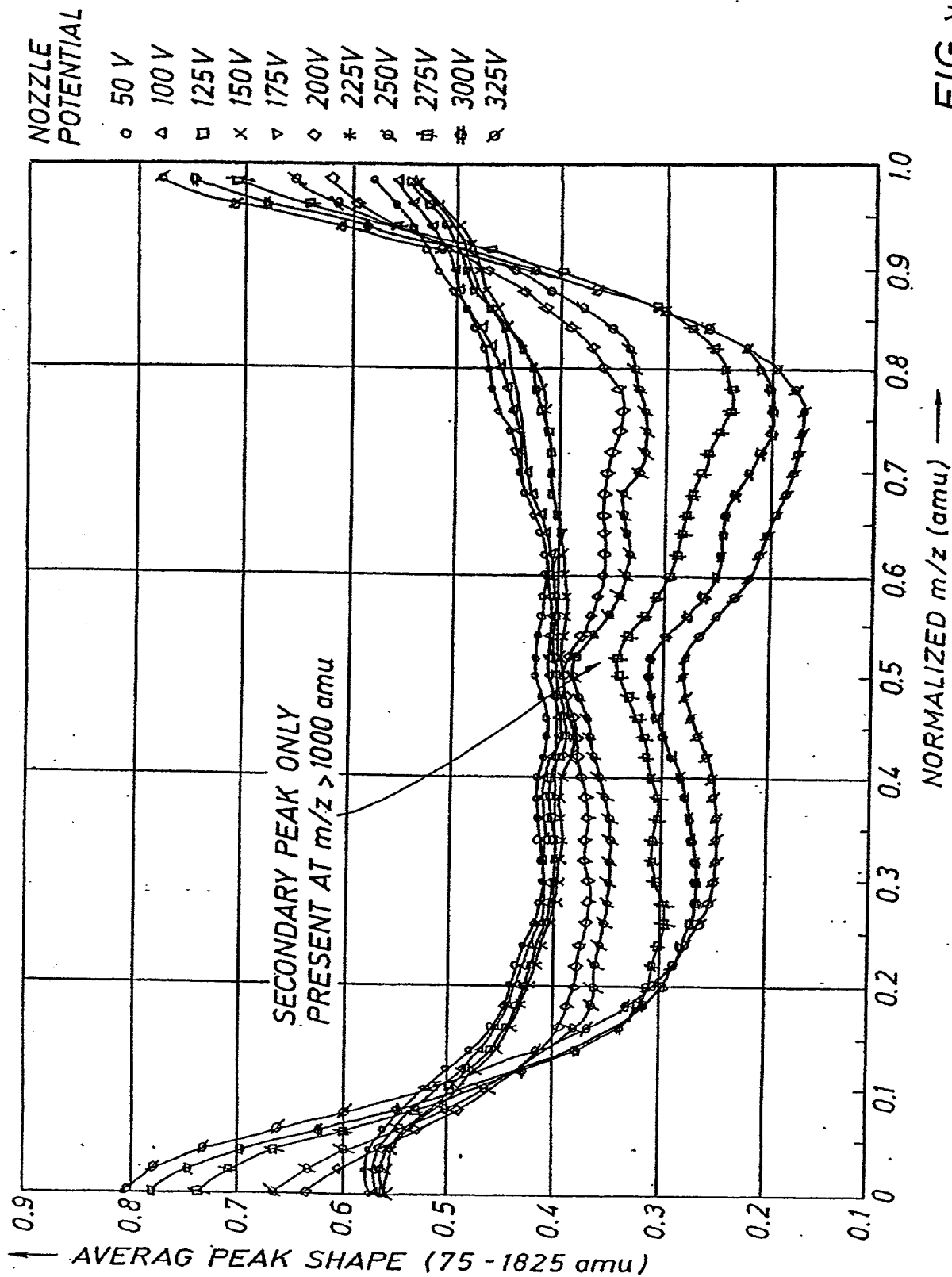


FIG. 16

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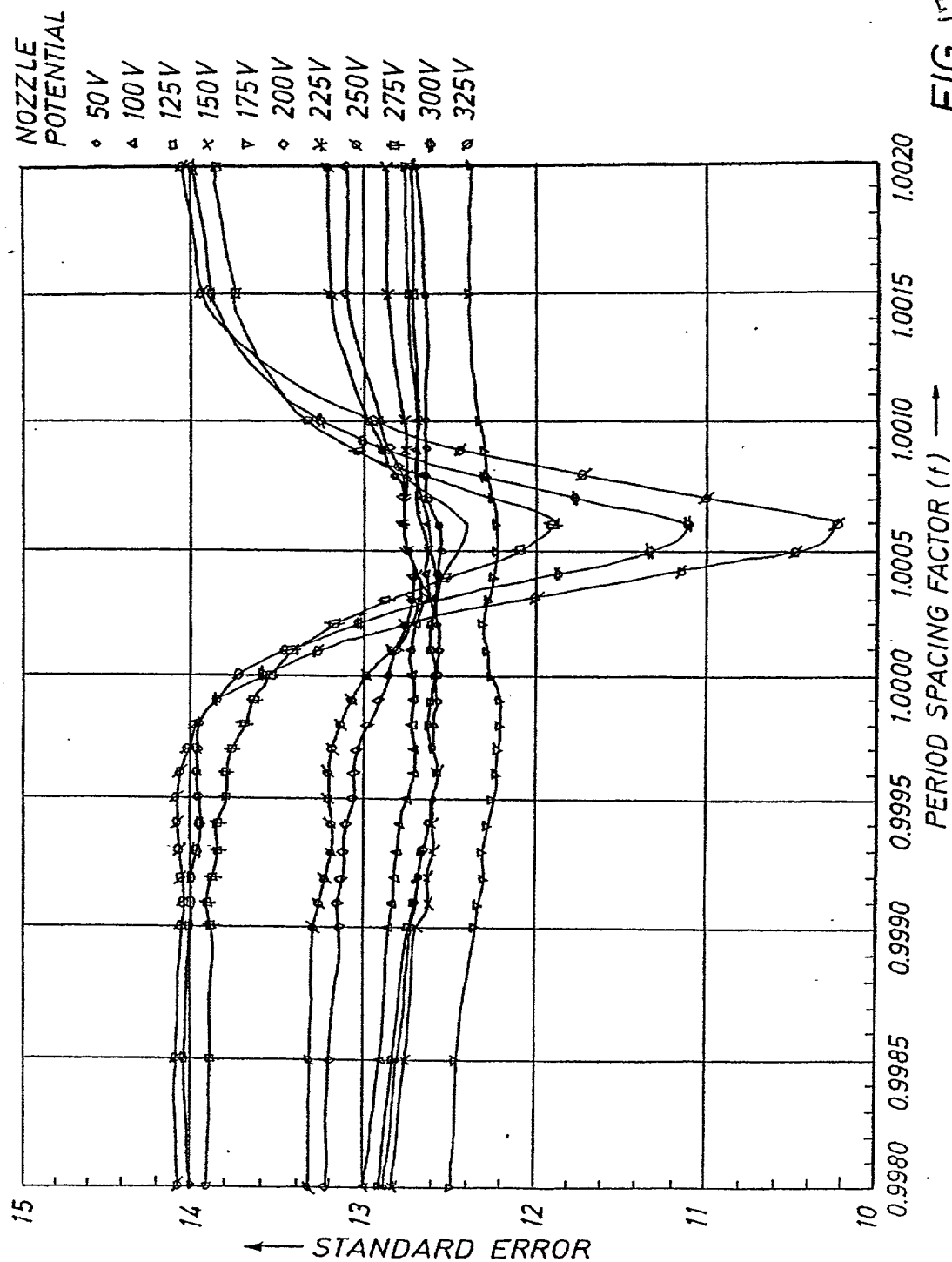
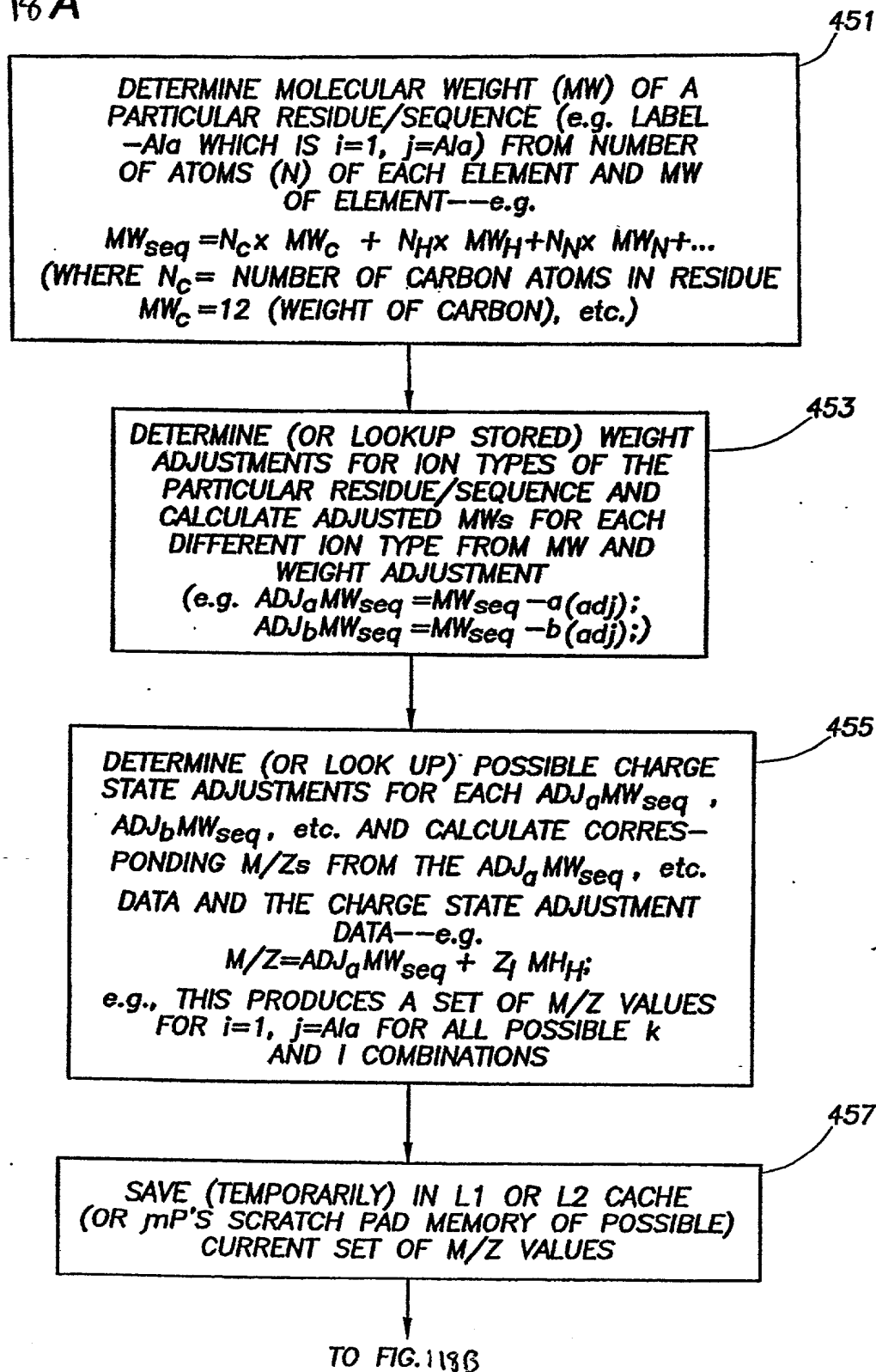


FIG. 17

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FIG. 18'A



FROM FIG. 18A

459  
PERFORM LOOKUP IN MASS SPECTRUM DATA  
AT EACH M/Z VALUE IN THE SAVED CURRENT  
SET OF M/Z VALUES TO OBTAIN ABUNDANCE  
VALUE AT EACH M/Z

461  
ERASE CURRENT SET OF M/Z VALUES IN  
CACHE (NOTE: MAY ERASE BY WRITING  
NEW CURRENT SET IN LATER ITERATION)

463  
REPEAT M/Z CALCULATIONS FOR NEXT POSSIBLE  
SEQUENCE (AND REPEAT M/Z CALCULATIONS  
FOR ALL OTHER POSSIBLE TERMINAL SEQUENCES  
UP TO n AAs IN LENGTH)  
(RETURN TO 451)

FIG. 18B

FIG. 19

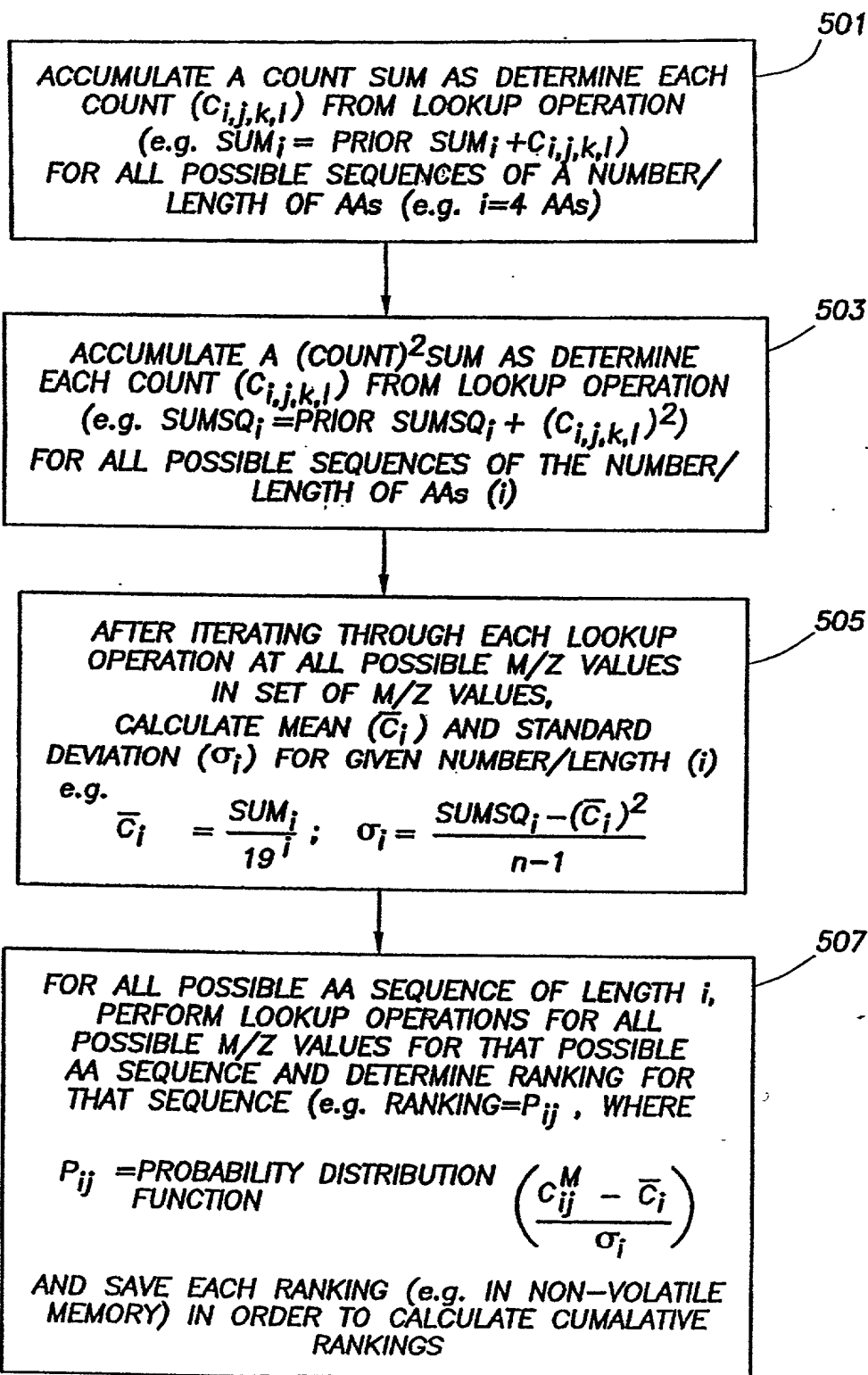


FIG. 19

FIG. 20A

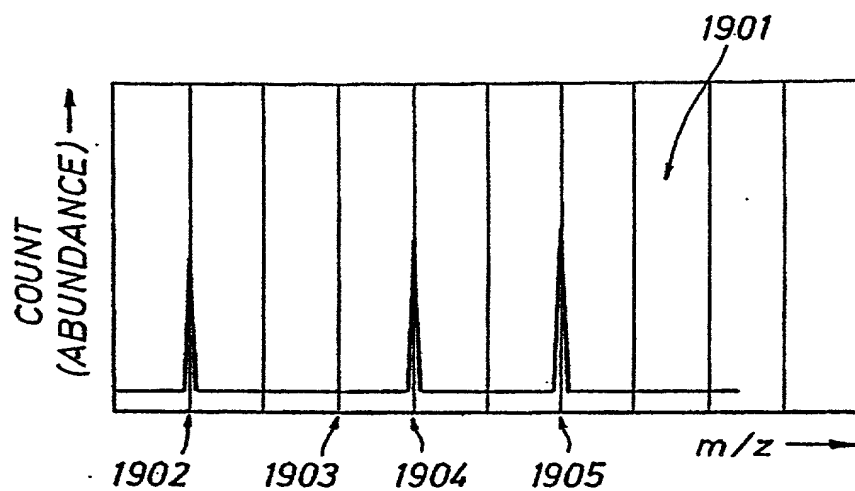
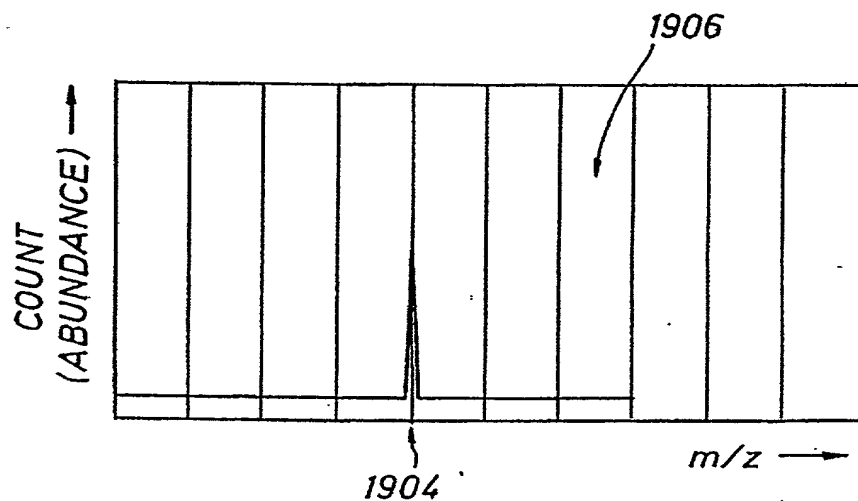


FIG. 120A.B



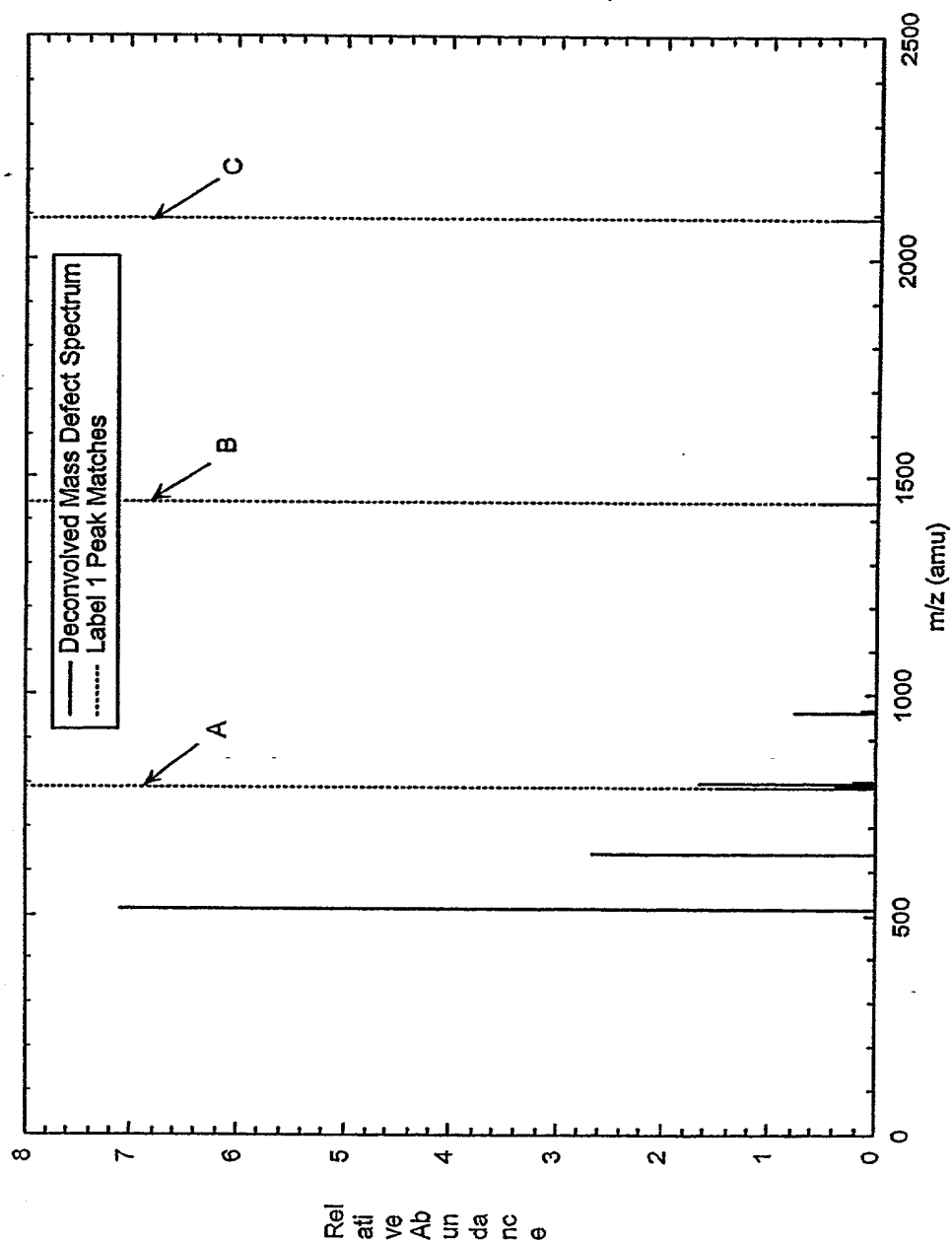


FIG. 21

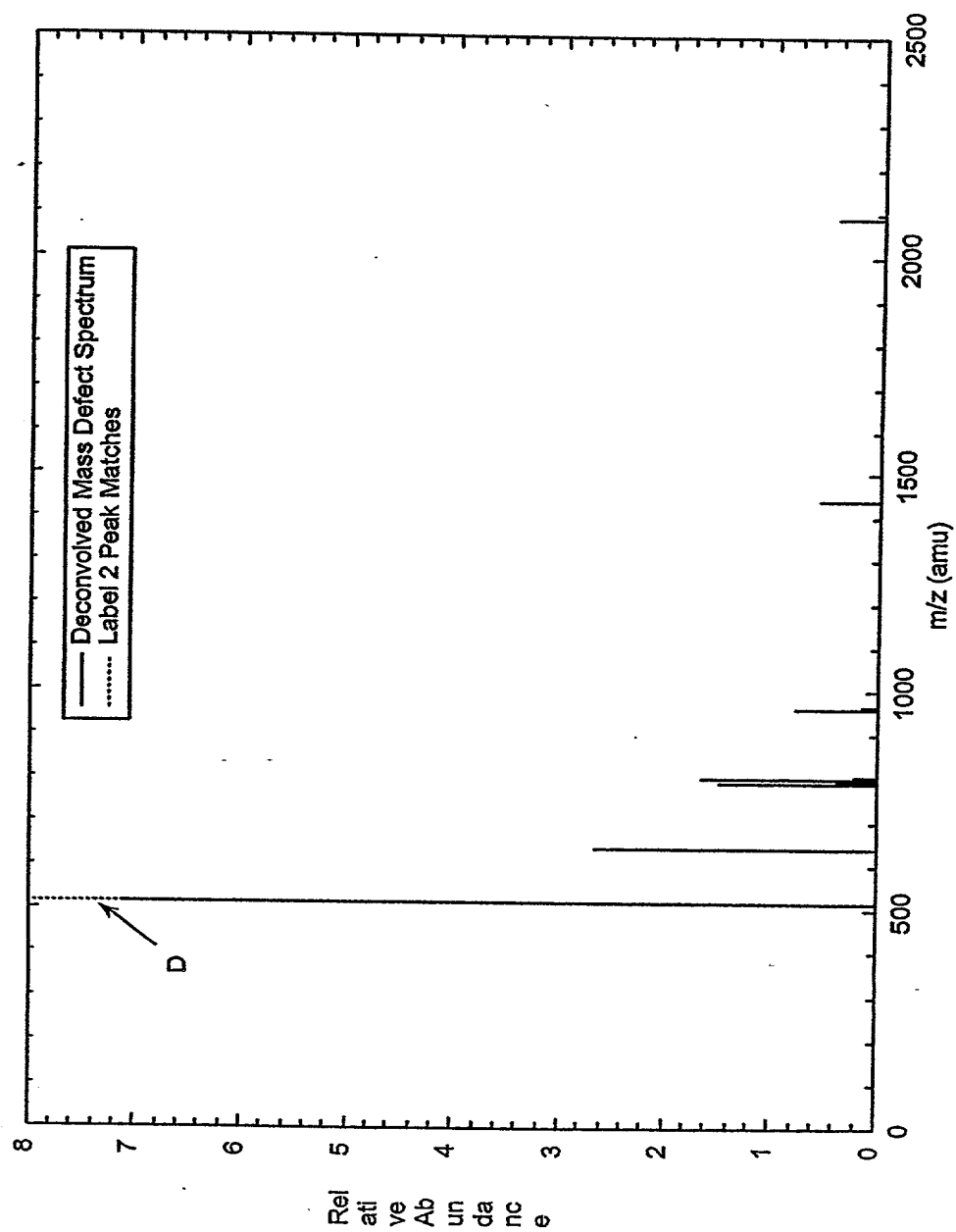


FIG. 22



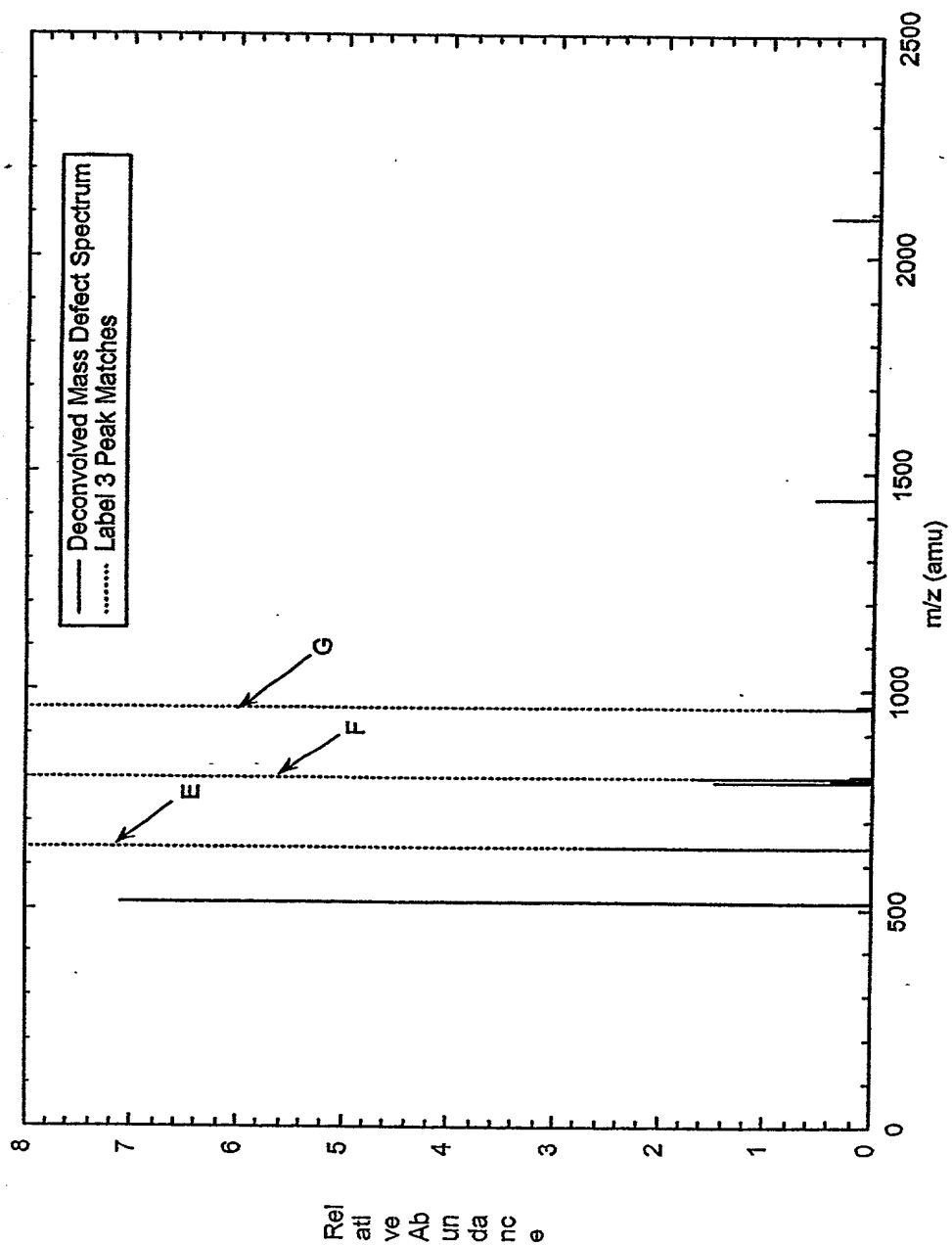


FIG. 2'3

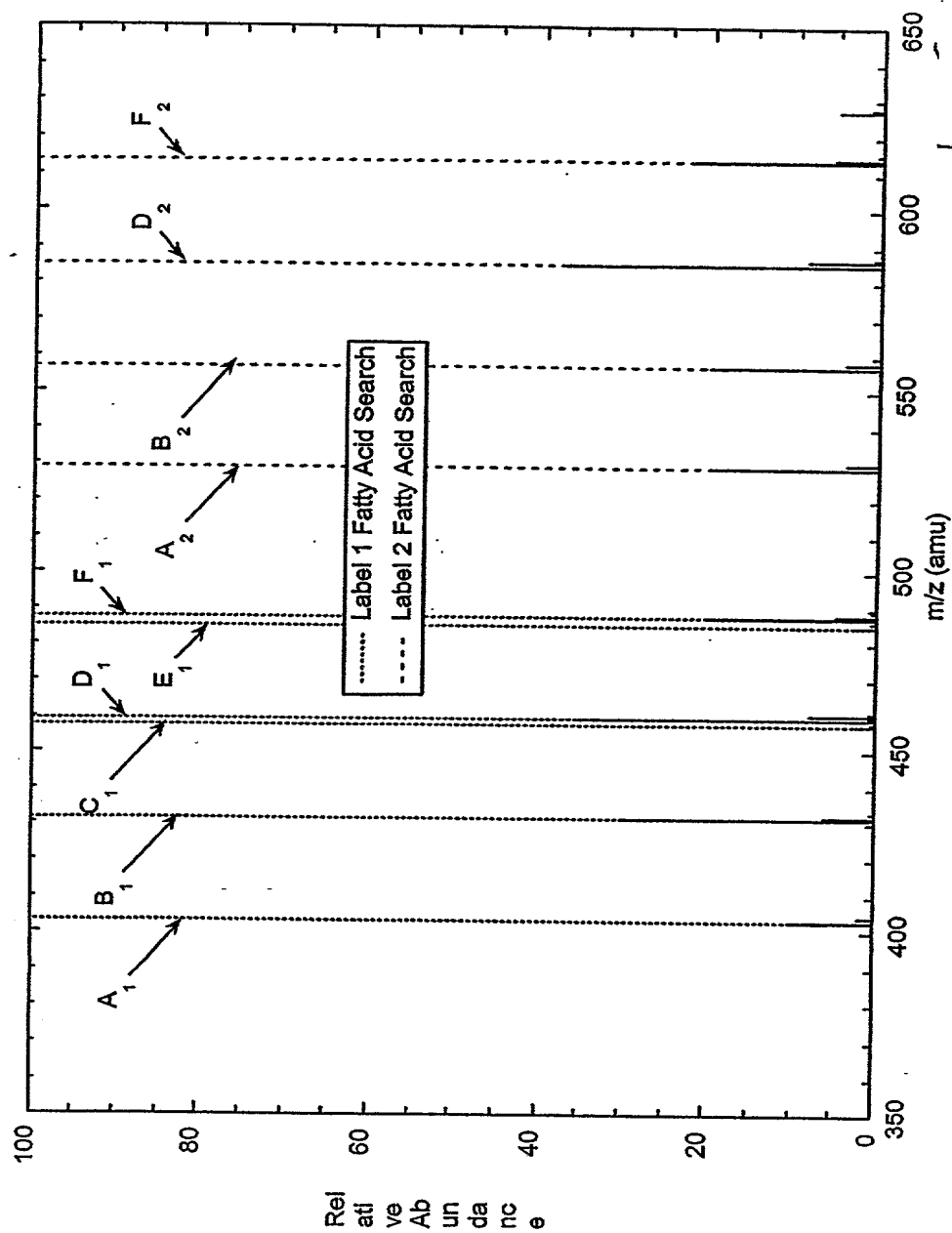
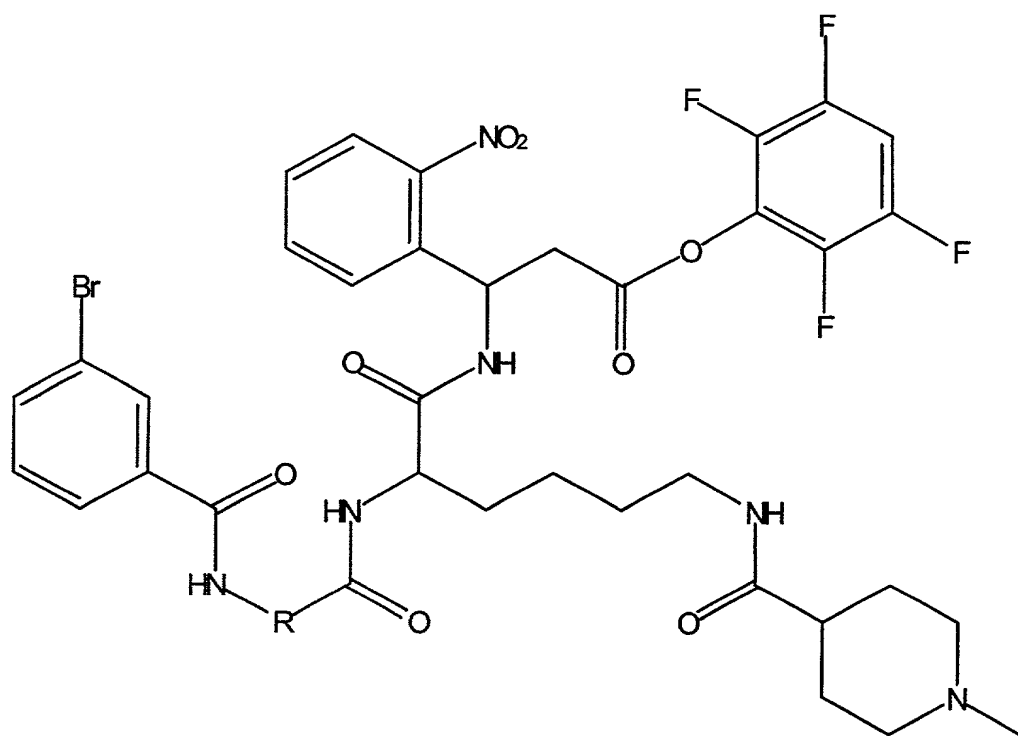


FIG. 2.4



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The general structure of the photocleavable mass defect tag where Br is the mass defect element that is linked through the amino acid (R) to the remainder of the tag.

FIG. 25

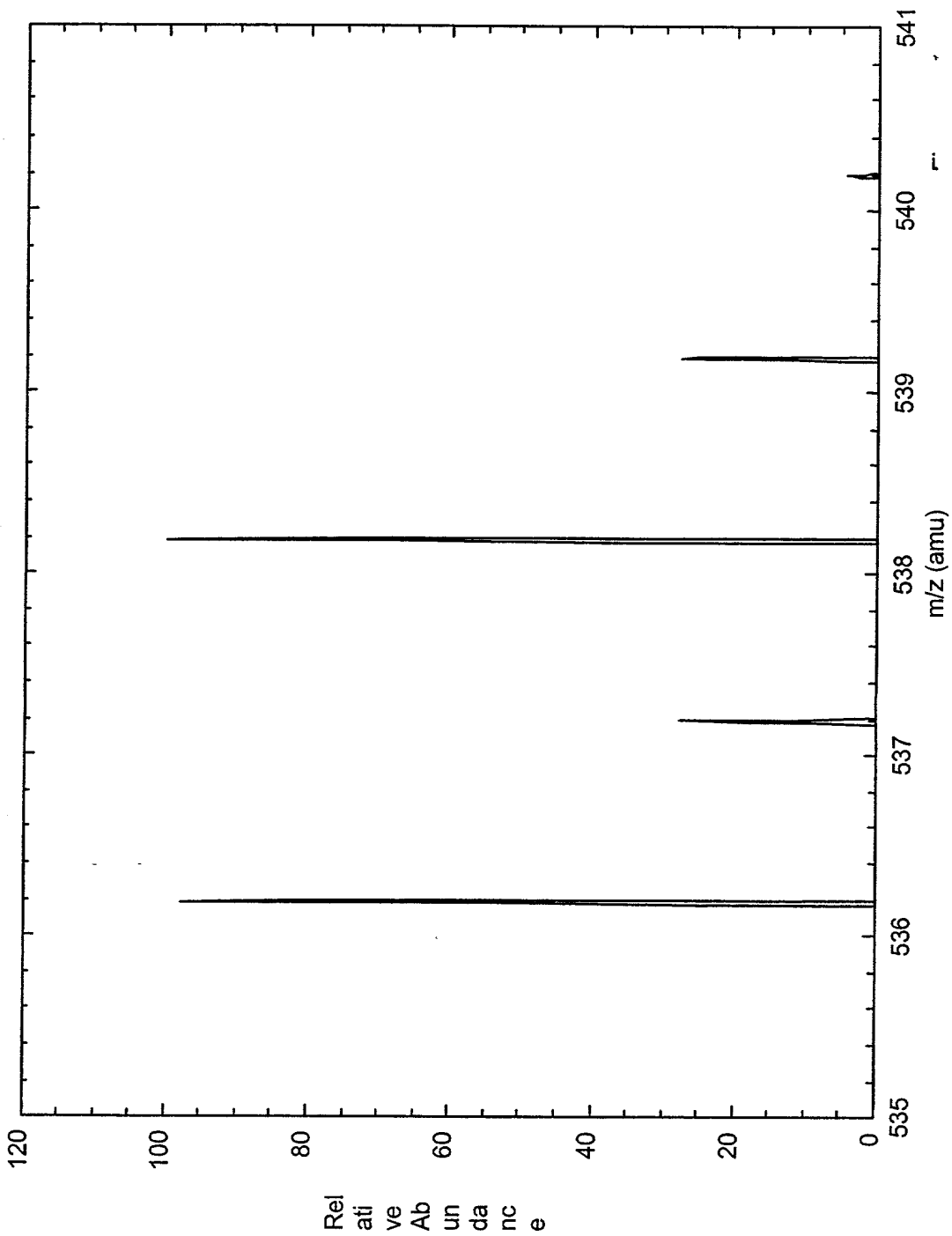


FIG 26

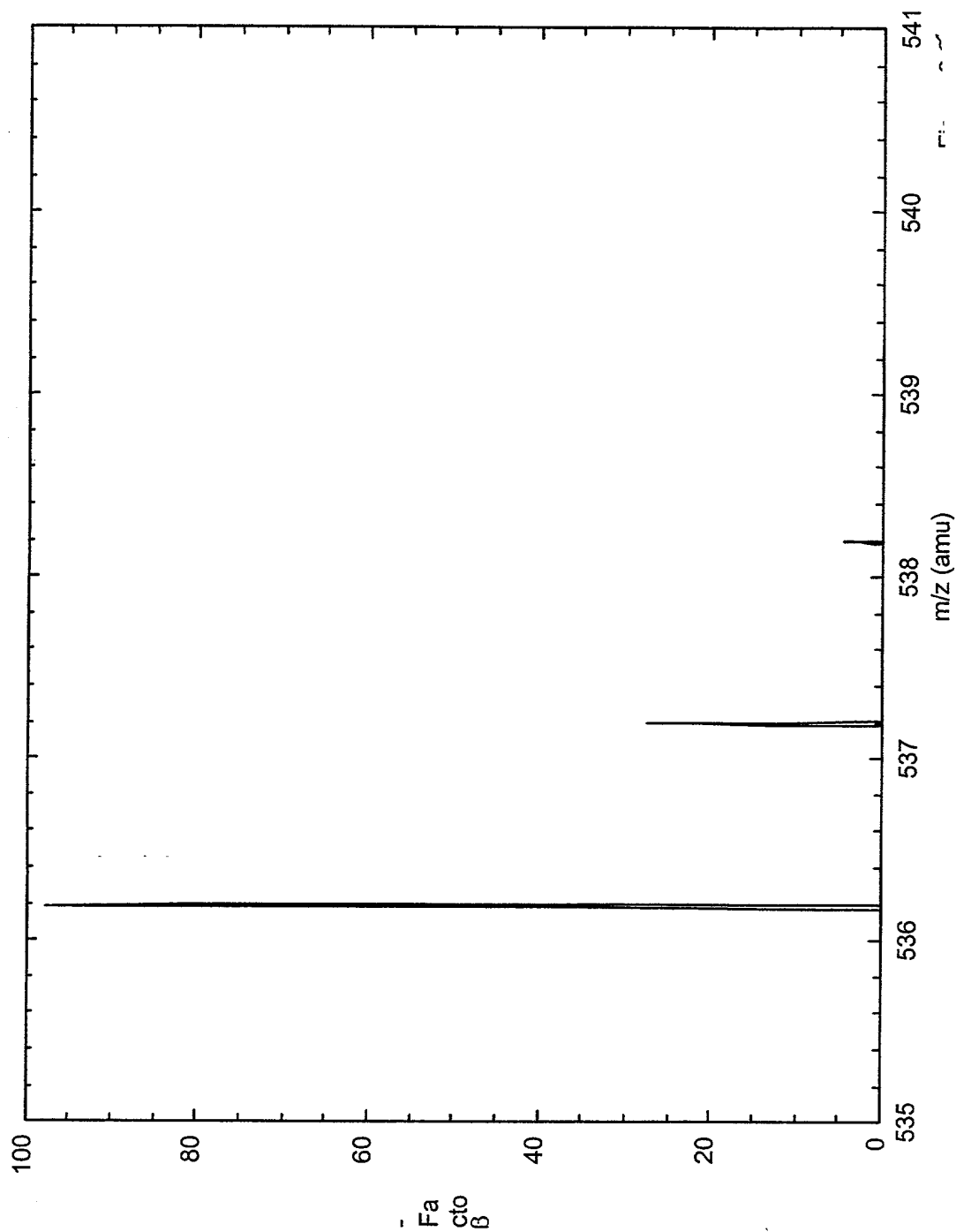


FIG 27

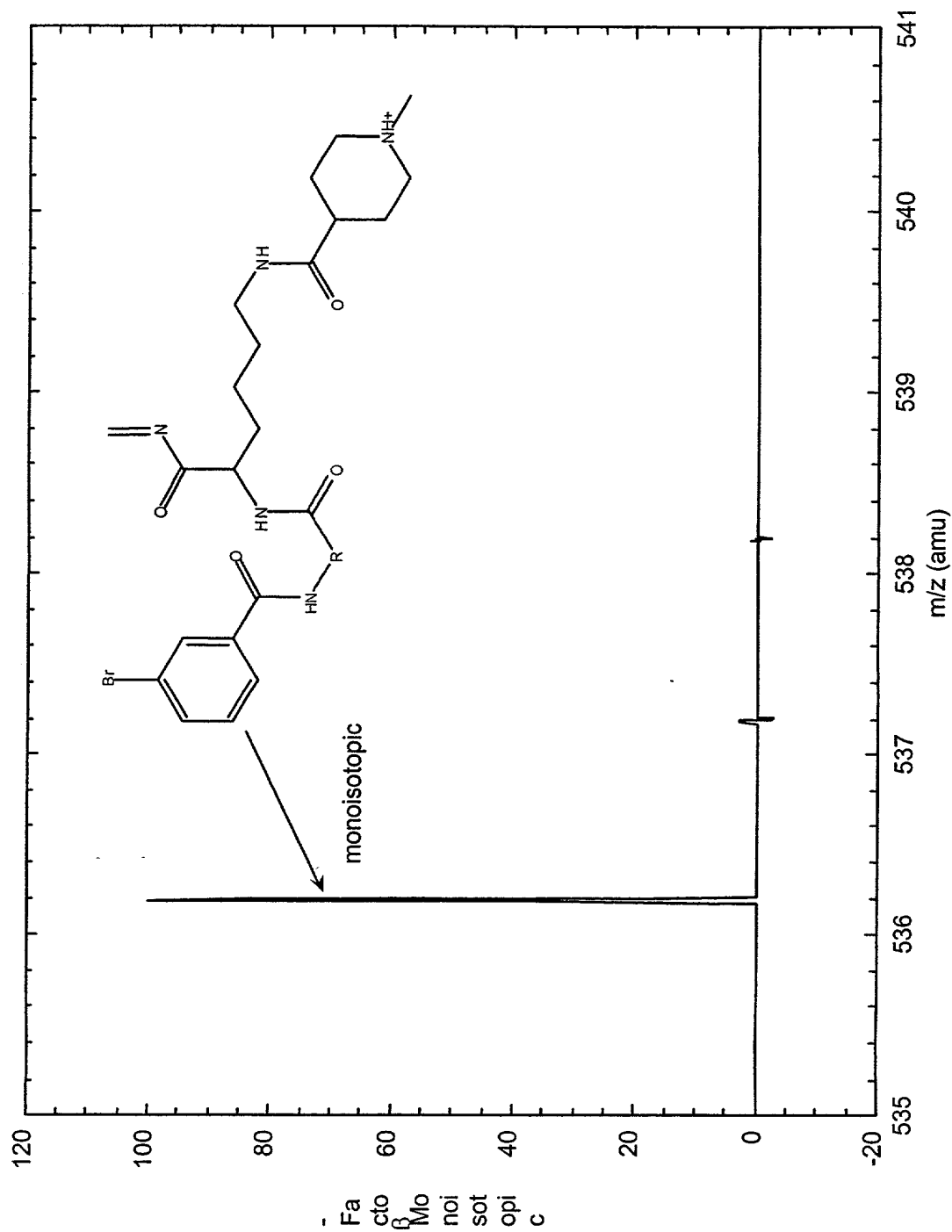


FIG 28

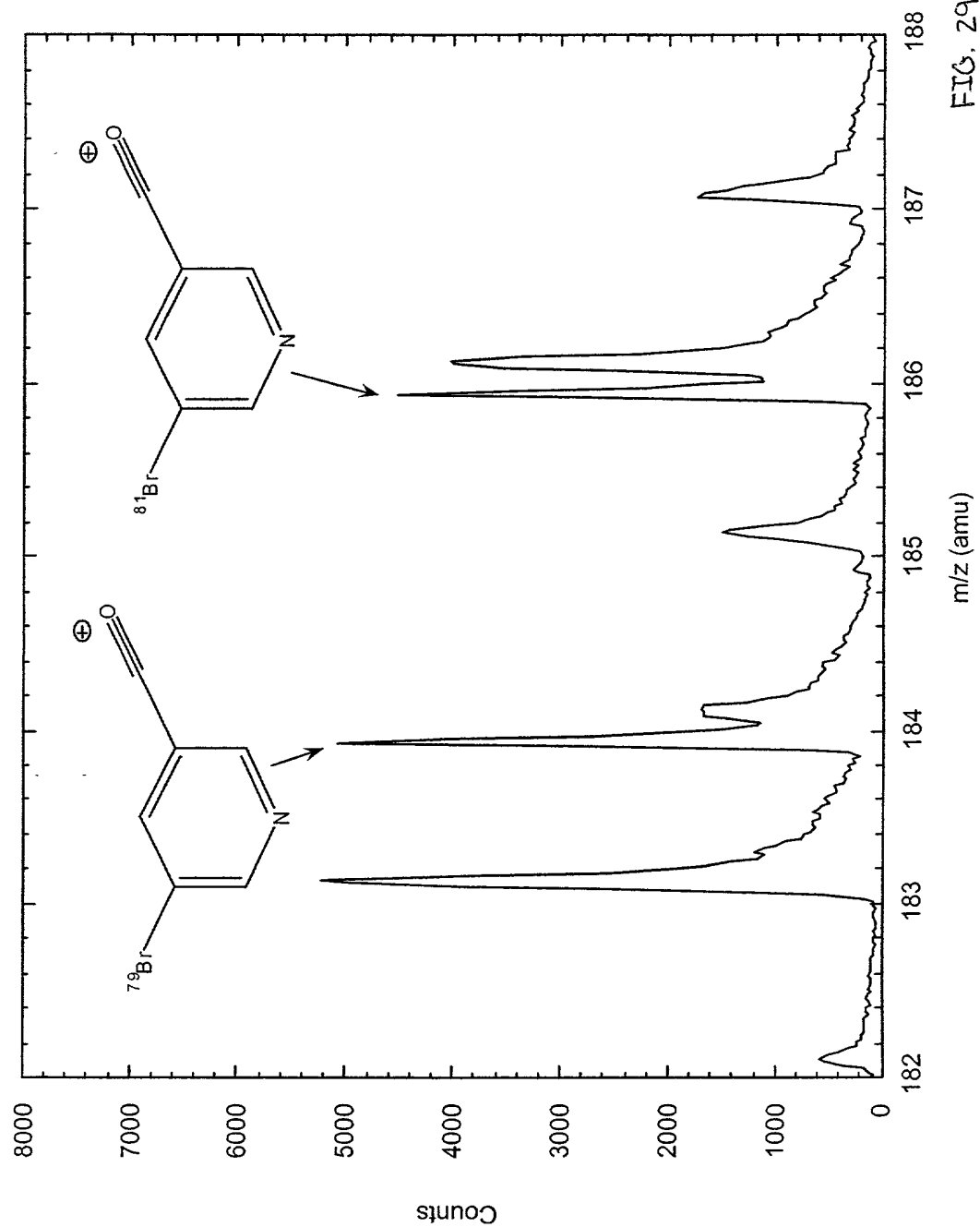


FIG. 29

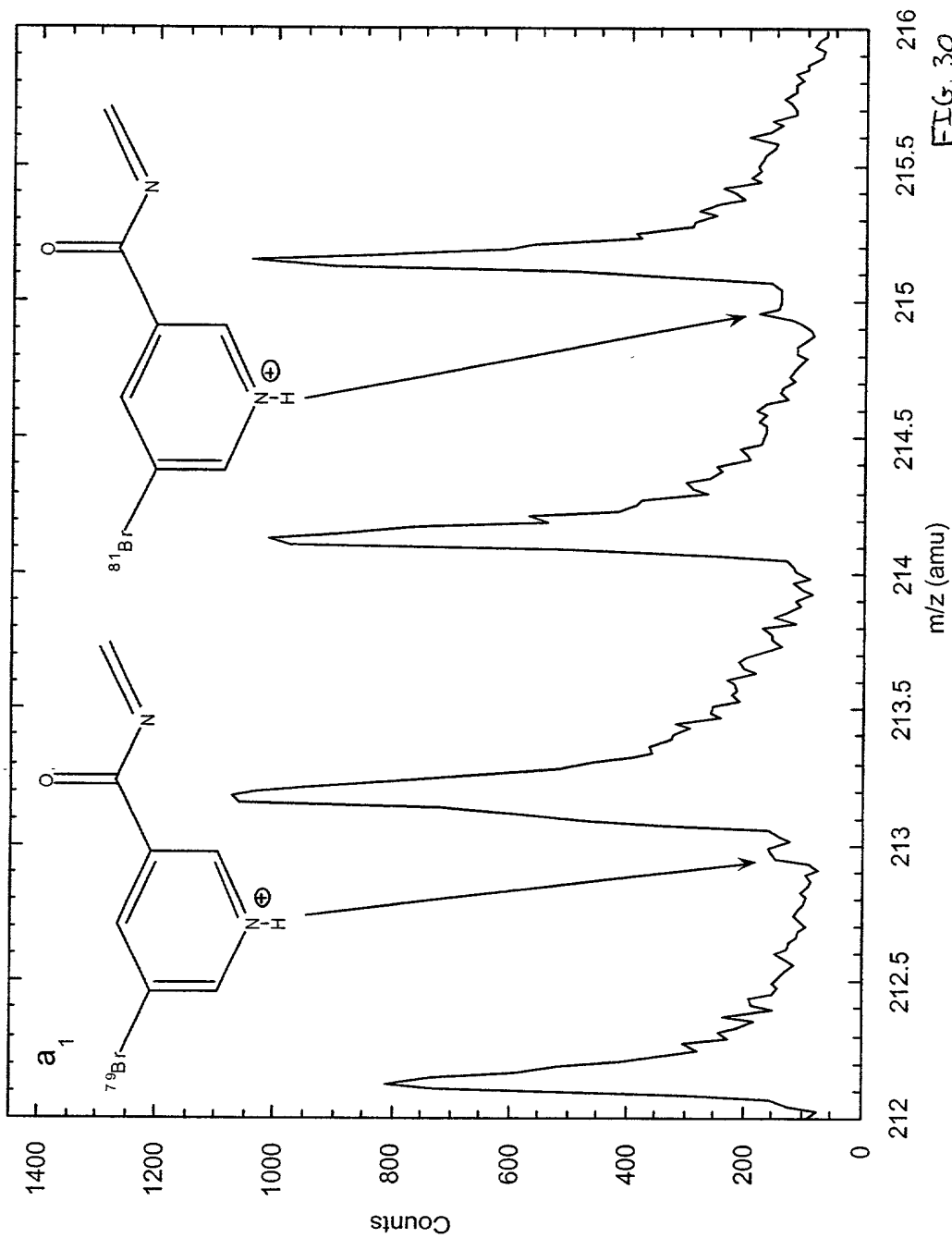


FIG. 30



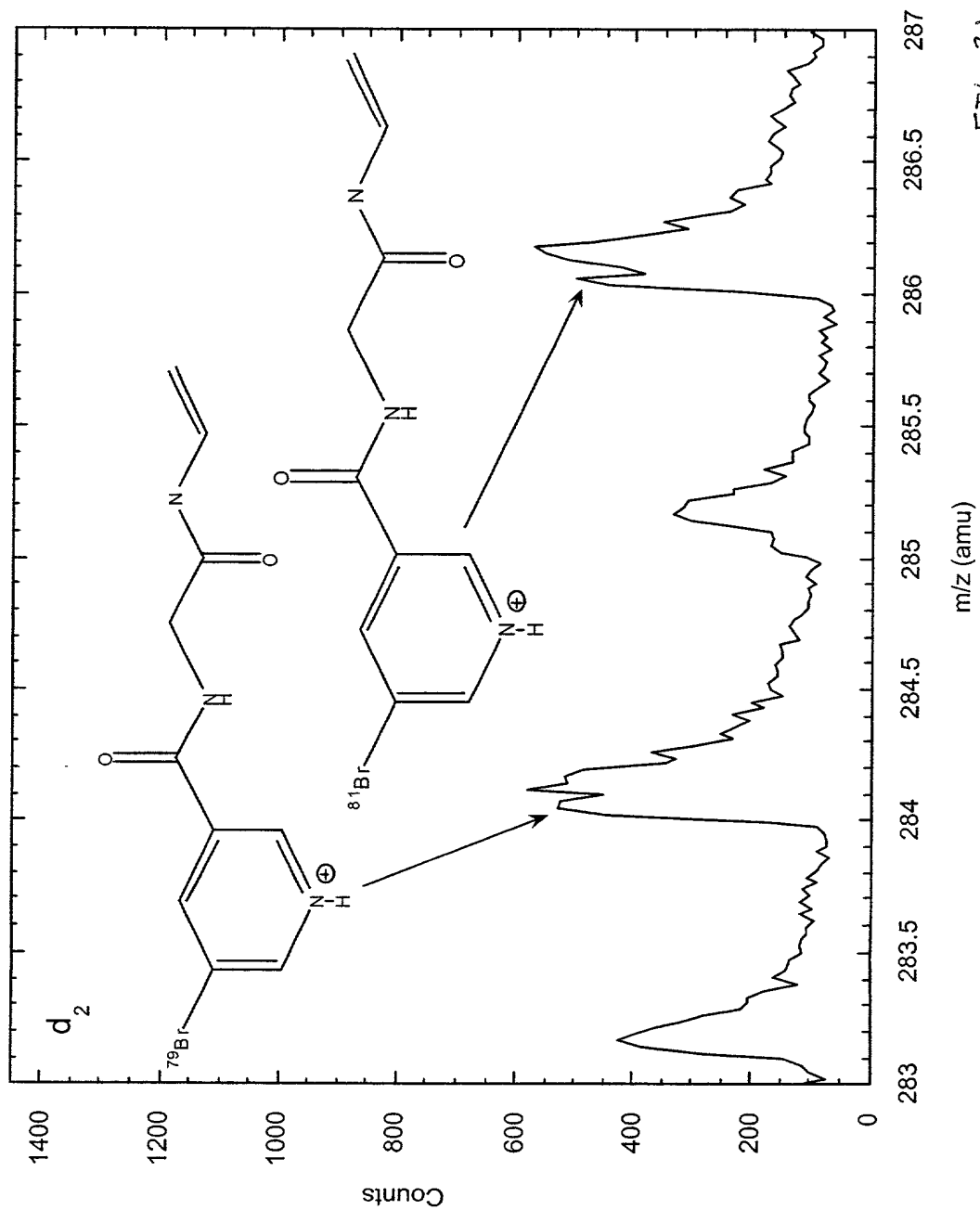
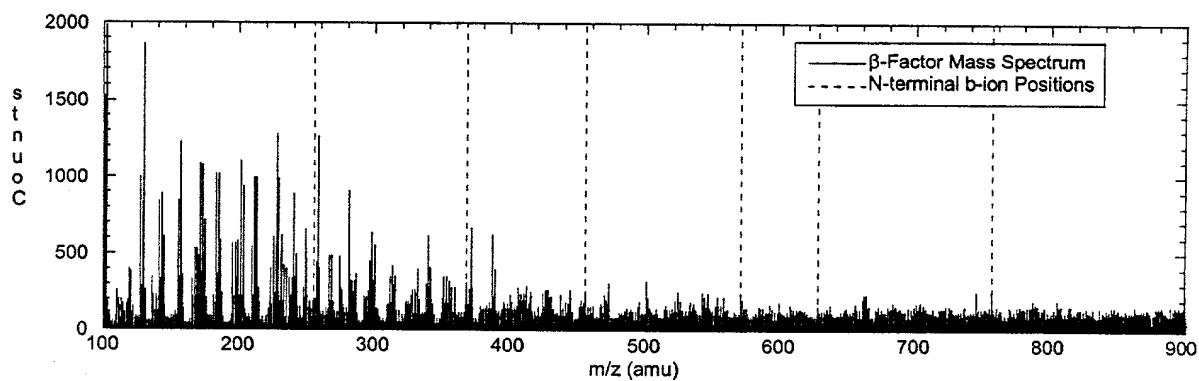
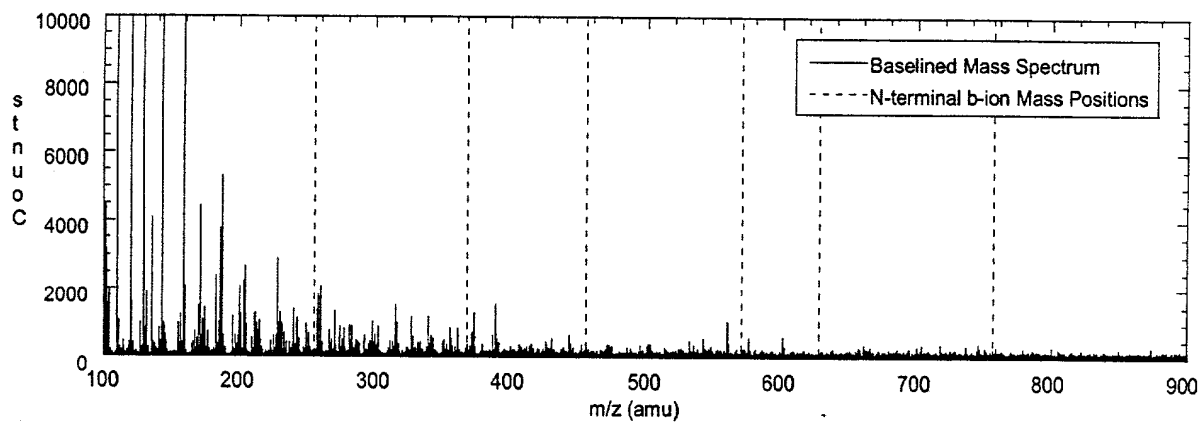
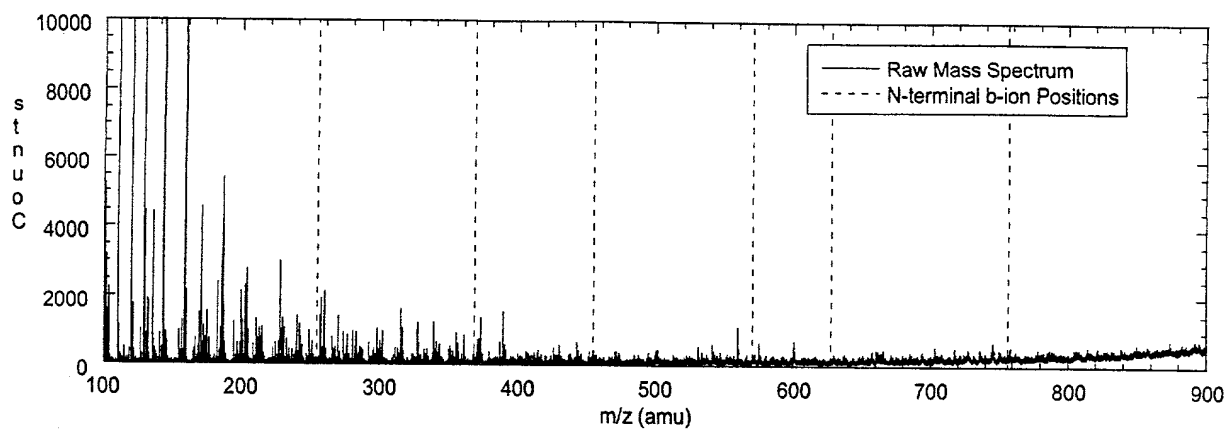


FIG. 31

Fig. 3.2



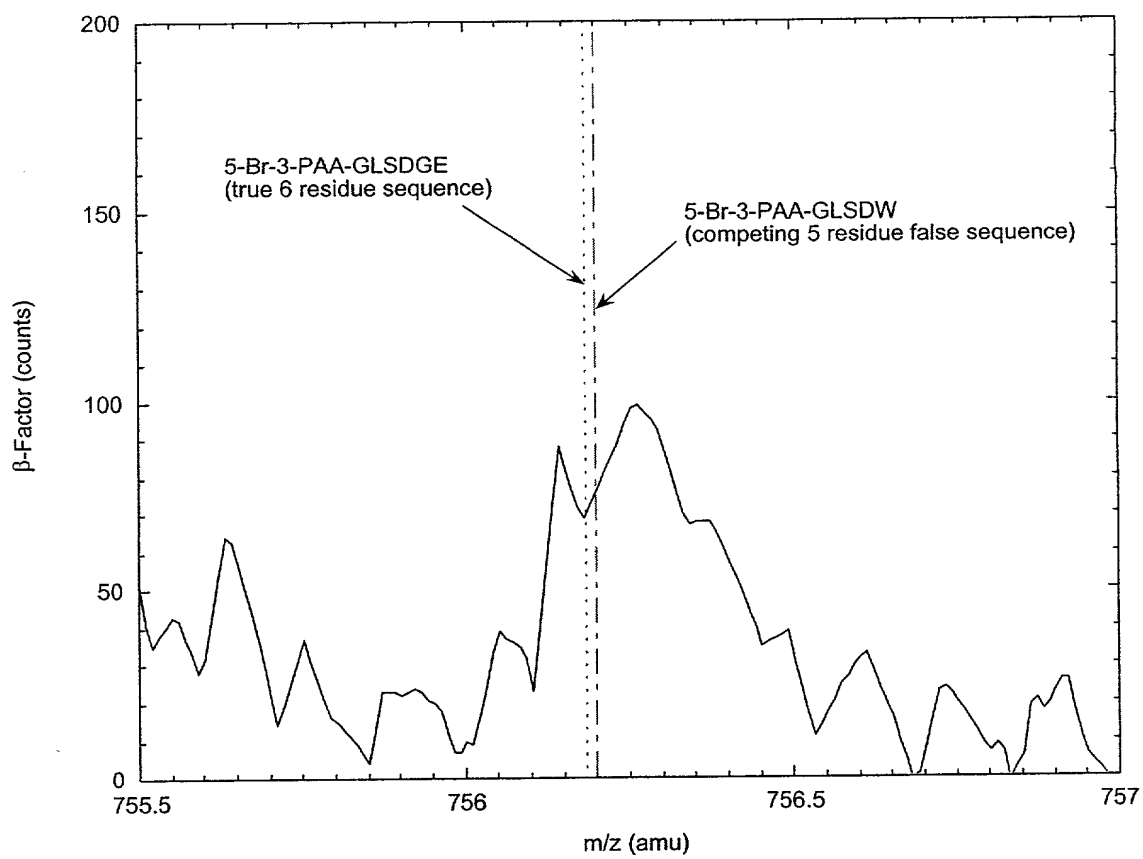


FIG. 33

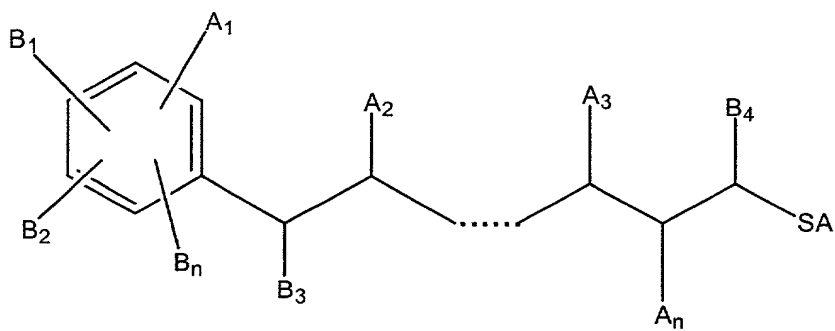


FIG. 34

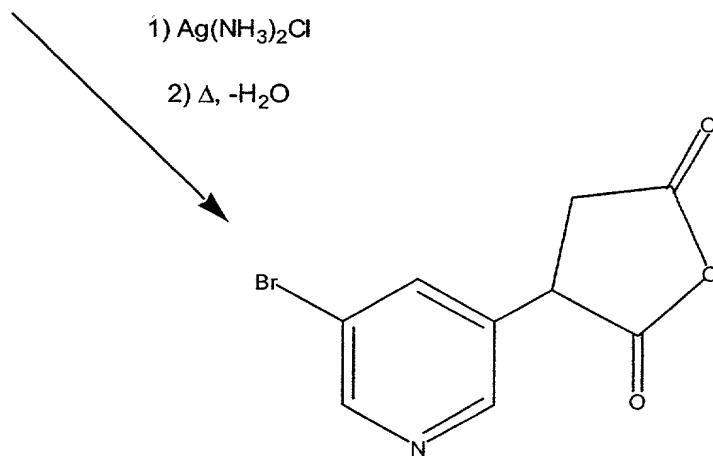
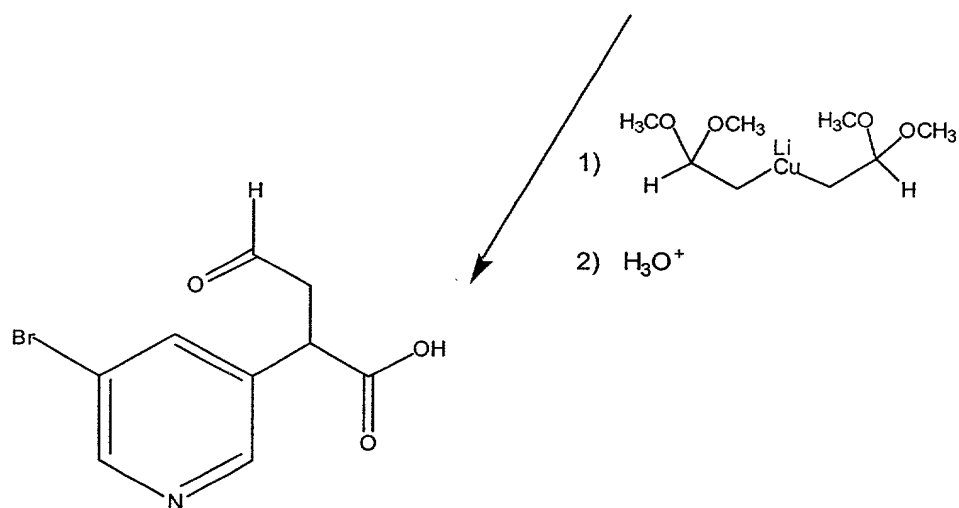
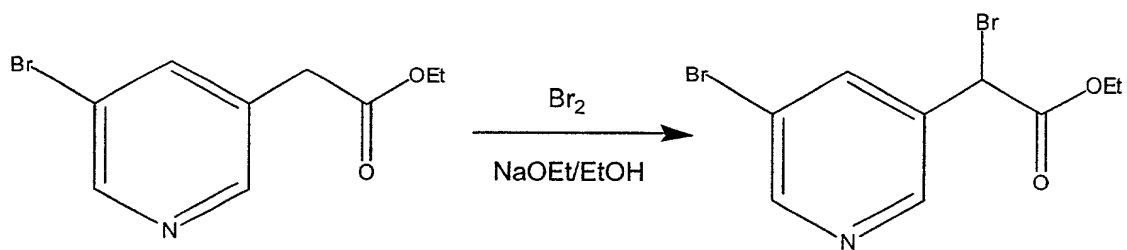


FIG. 35



M13 primer

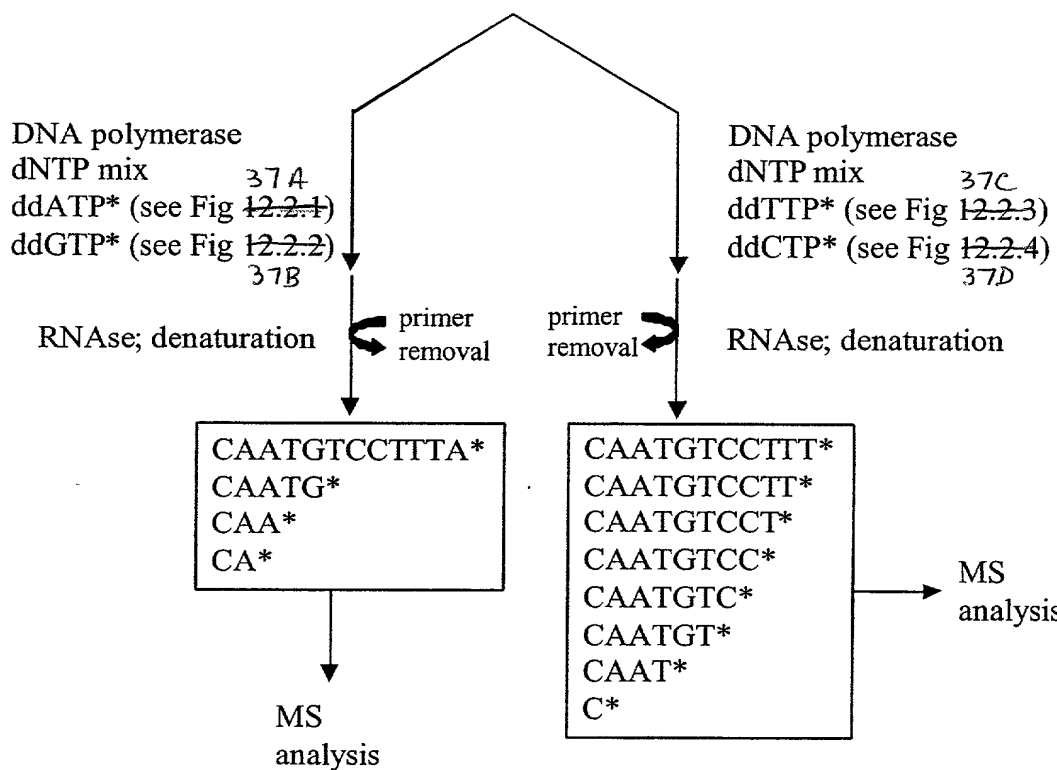
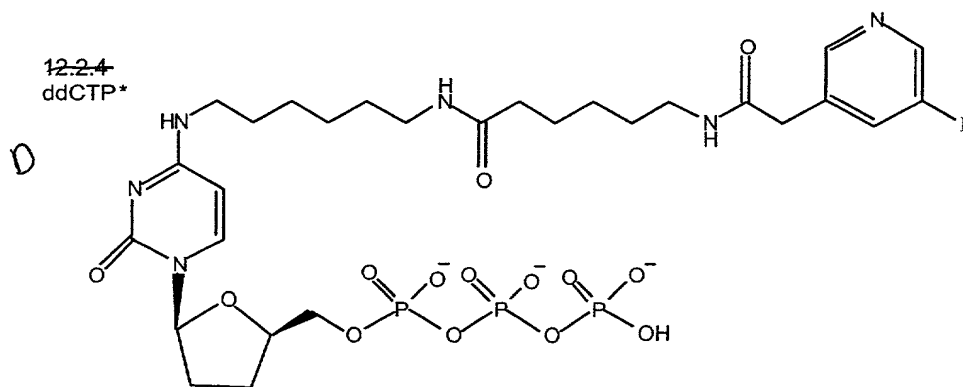
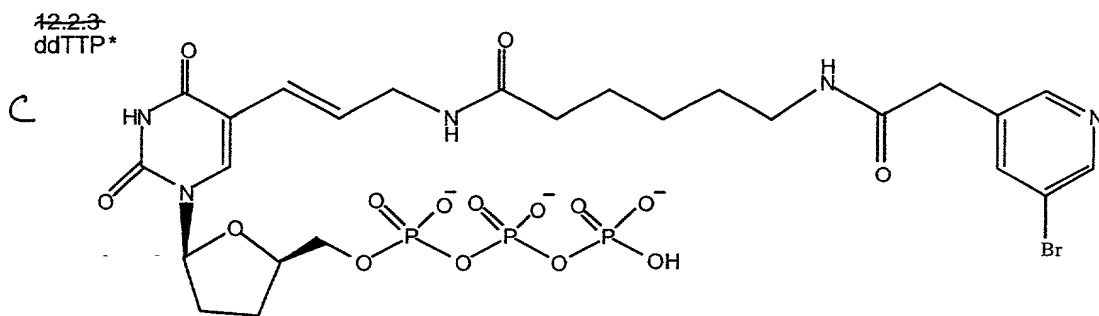
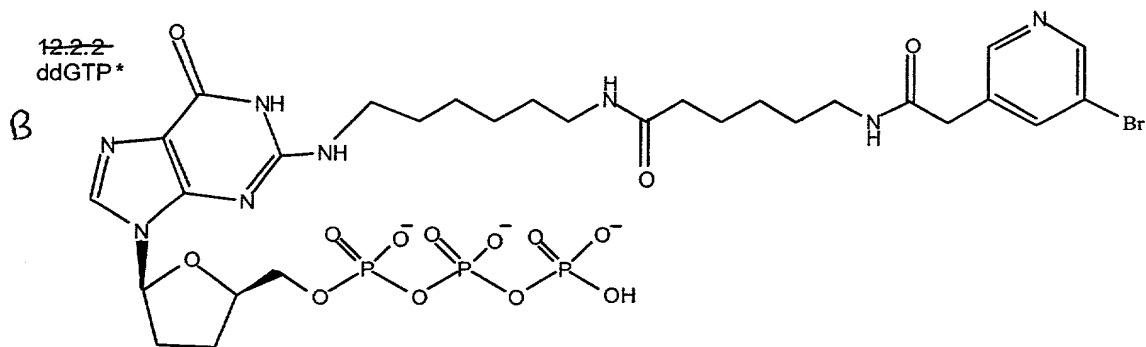
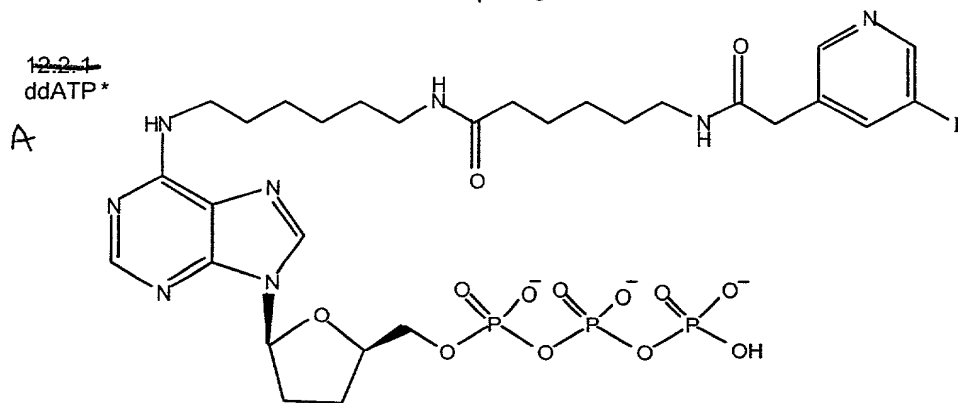


FIG. 36

FIG. 37



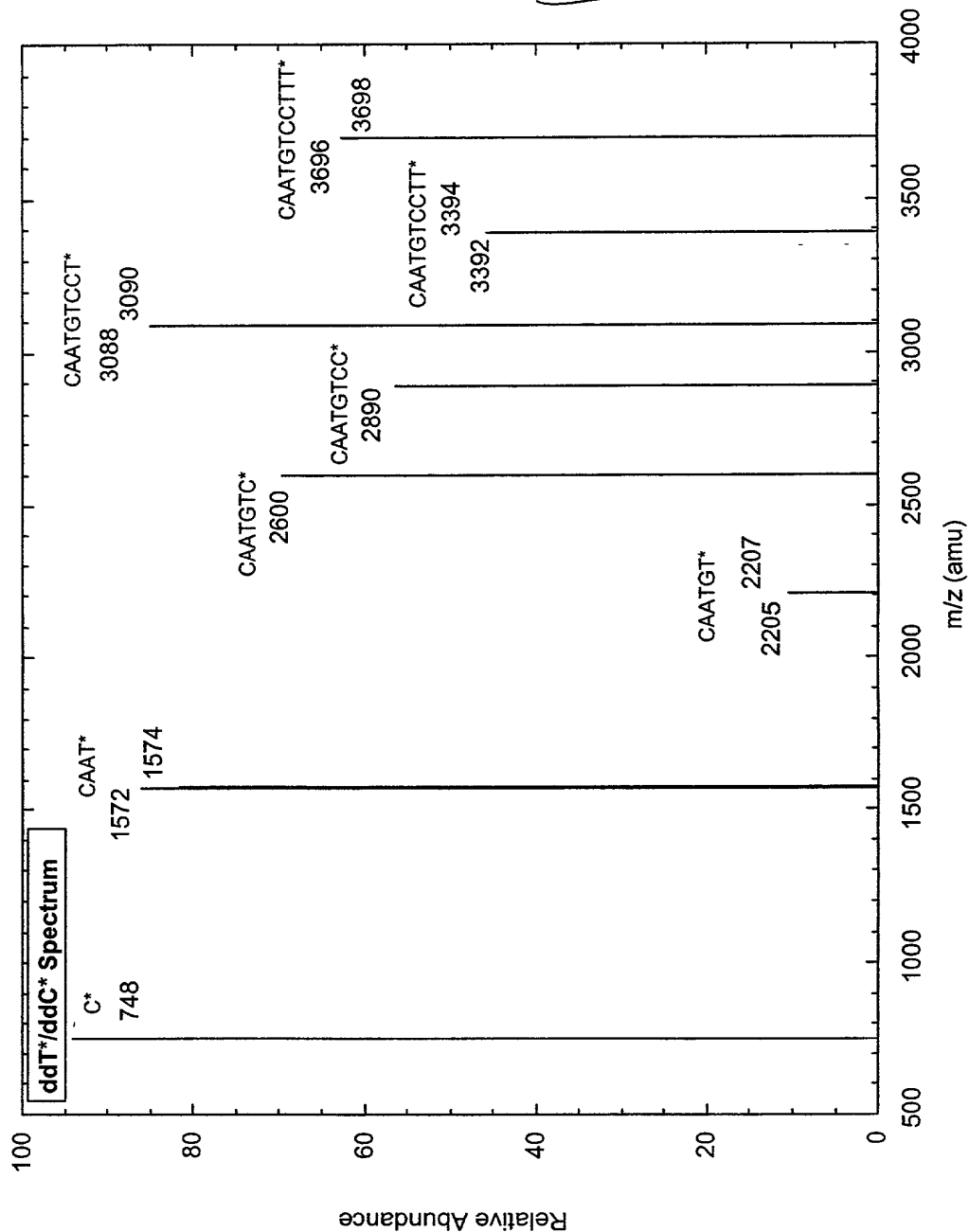


Fig. 39



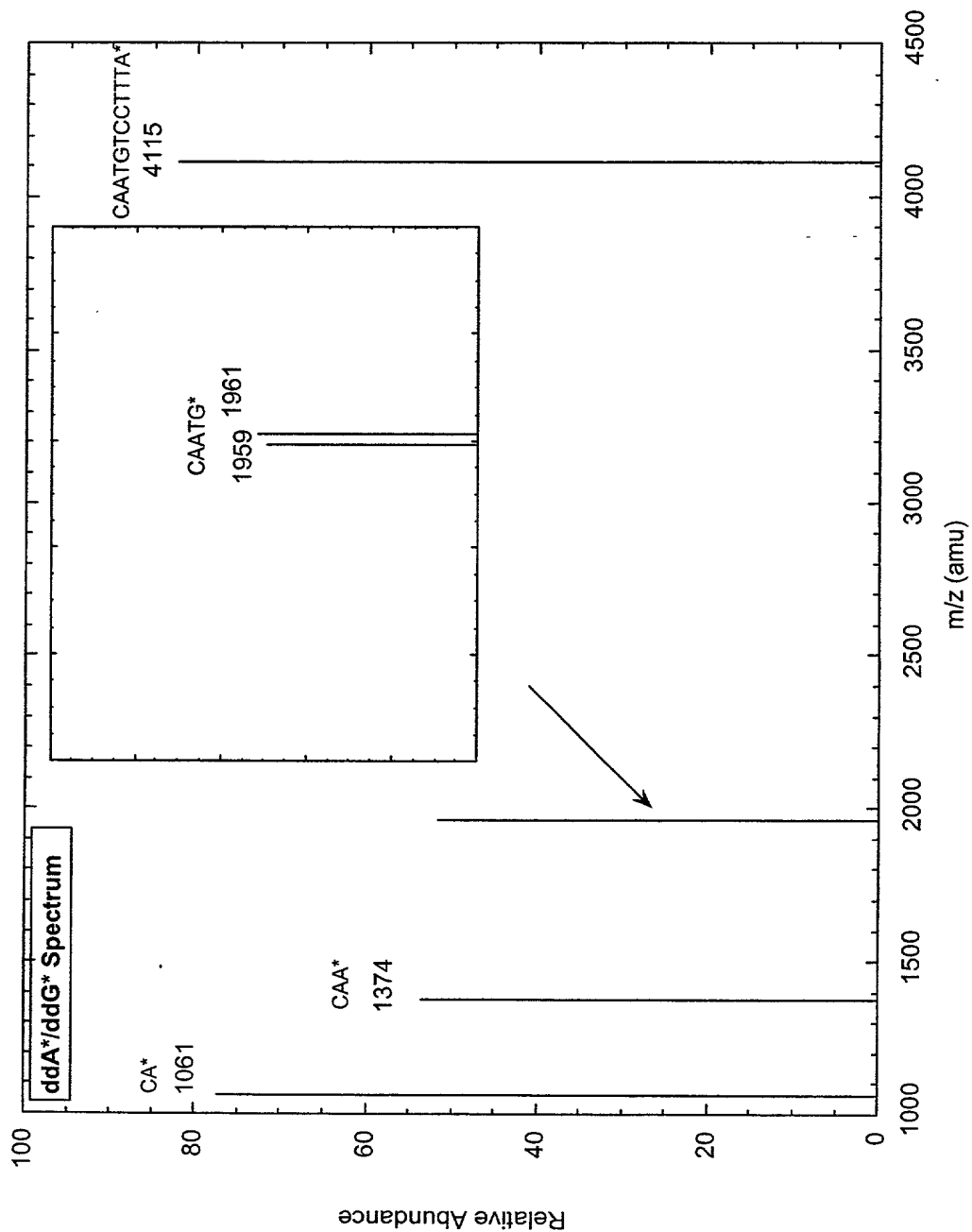


FIG. 38